



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:35 AM UTC

PDB ID : 2GBF / pdb_00002gbf
Title : rat dpp-IV with alkynyl cyanopyrrolidine #1
Authors : Longenecker, K.L.; Jakob, C.G.; Fry, E.H.; Wilk, S.
Deposited on : 2006-03-10
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

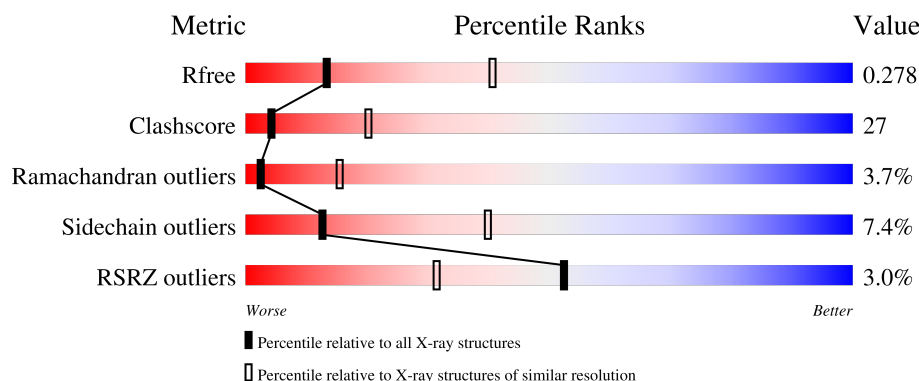
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

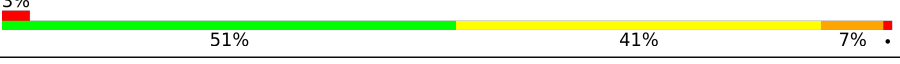
The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	730	
1	B	730	

2 Entry composition [i](#)

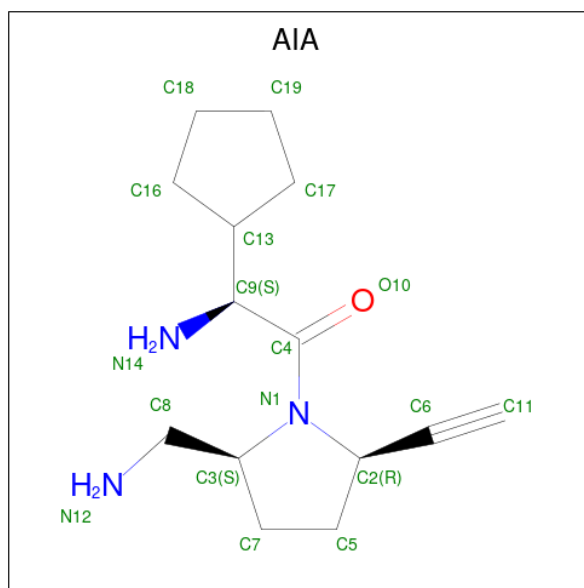
There are 2 unique types of molecules in this entry. The entry contains 11858 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5920	3789	981	1124	26			
1	B	730	Total	C	N	O	S	0	0	0
			5920	3789	981	1124	26			

- Molecule 2 is (1S)-2-[(2S,5R)-2-(AMINOMETHYL)-5-ETHYNYLPYRROLIDIN-1-YL]-1-CYCLOPENTYL-2-OXOETHANAMINE (CCD ID: AIA) (formula: $C_{14}H_{23}N_3O$).

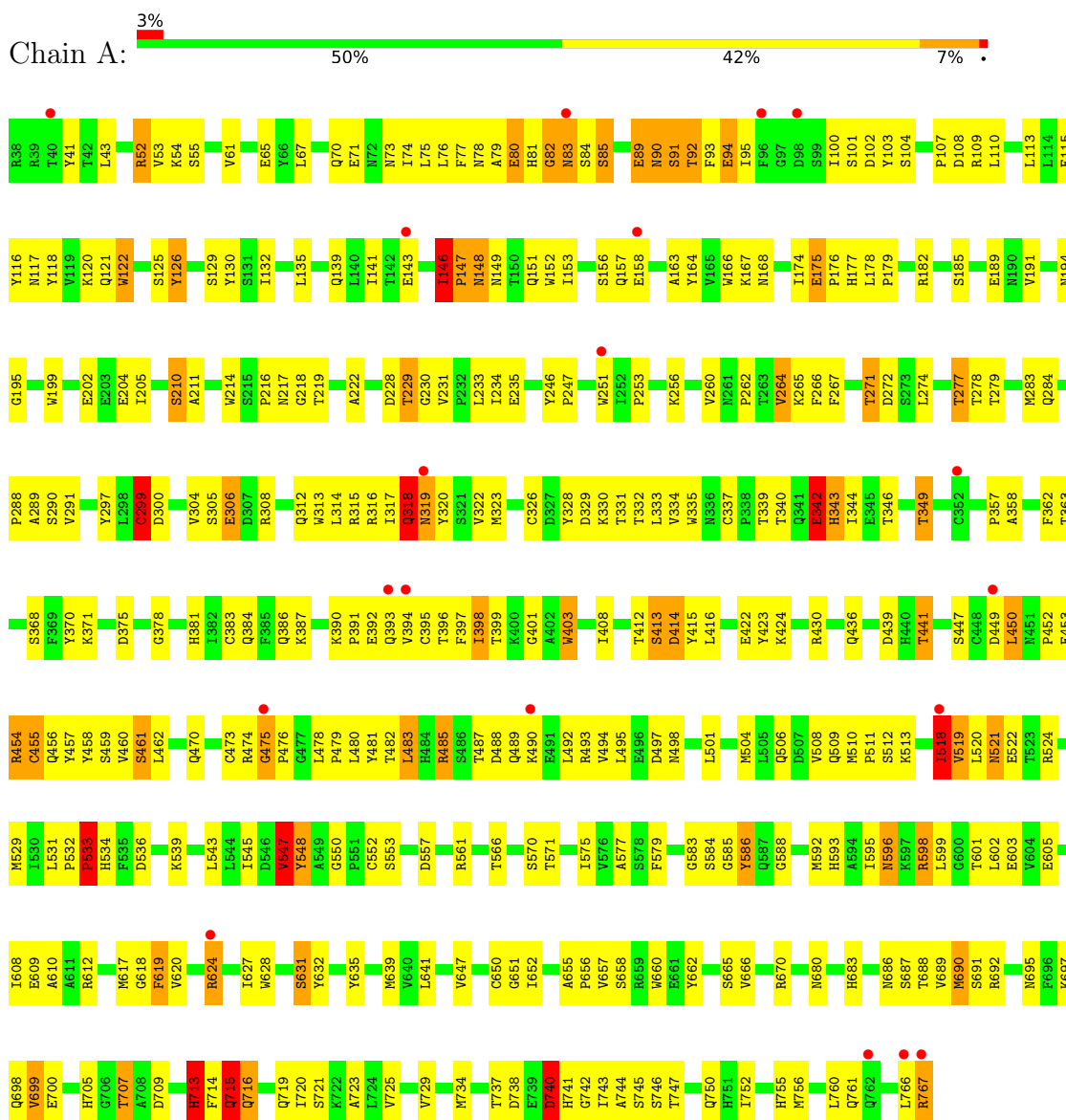


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	14	3	1		

3 Residue-property plots

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

• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	208.17Å 208.17Å 208.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.10) 98.9 (20.00-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.289 0.243 , 0.278	Depositor DCC
R_{free} test set	2743 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11858	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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

5.1 Standard geometry

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

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	0.56	1/6088 (0.0%)	1.07	45/8278 (0.5%)
1	B	0.51	1/6088 (0.0%)	1.06	43/8278 (0.5%)
All	All	0.53	2/12176 (0.0%)	1.07	88/16556 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	631	SER	C-O	12.89	1.40	1.24
1	B	283	MET	SD-CE	5.65	1.93	1.79

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ASN	N-CA-C	-11.45	97.10	111.75
1	B	90	ASN	N-CA-C	-11.38	97.18	111.75
1	B	713	HIS	N-CA-C	9.33	130.67	110.80
1	A	713	HIS	N-CA-C	9.25	130.50	110.80
1	B	474	ARG	N-CA-C	-8.74	102.62	113.38
1	A	278	THR	N-CA-C	-8.61	101.62	112.90
1	B	278	THR	N-CA-C	-8.36	101.94	112.90
1	A	474	ARG	N-CA-C	-8.29	102.94	113.72
1	B	89	GLU	N-CA-C	7.73	121.80	110.59
1	A	89	GLU	N-CA-C	7.72	121.95	110.52
1	B	715	GLN	N-CA-C	-7.14	102.61	111.75
1	A	665	SER	N-CA-C	7.01	118.61	110.97
1	B	547	VAL	N-CA-C	7.00	119.62	108.85
1	A	43	LEU	N-CA-C	-6.99	104.01	112.54
1	B	43	LEU	N-CA-C	-6.87	104.16	112.54
1	A	715	GLN	N-CA-C	-6.82	103.02	111.75
1	B	455	CYS	N-CA-C	6.78	119.46	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	665	SER	N-CA-C	6.74	118.32	110.97
1	A	547	VAL	N-CA-C	6.72	119.20	108.85
1	B	146	ILE	CA-C-N	6.70	128.22	119.84
1	B	146	ILE	C-N-CA	6.70	128.22	119.84
1	A	204	GLU	N-CA-C	6.59	121.61	113.50
1	A	455	CYS	N-CA-C	6.58	119.14	108.41
1	A	660	TRP	N-CA-C	6.56	120.38	112.38
1	B	497	ASP	N-CA-C	-6.53	98.25	108.90
1	B	660	TRP	N-CA-C	6.49	120.30	112.38
1	A	319	ASN	N-CA-C	-6.49	104.29	111.36
1	B	459	SER	N-CA-C	-6.45	99.40	109.72
1	B	234	ILE	N-CA-C	-6.44	99.21	108.48
1	B	318	GLN	CA-C-N	6.38	129.34	120.29
1	B	318	GLN	C-N-CA	6.38	129.34	120.29
1	A	318	GLN	CA-C-N	6.36	129.32	120.29
1	A	318	GLN	C-N-CA	6.36	129.32	120.29
1	A	234	ILE	N-CA-C	-6.36	99.33	108.48
1	B	319	ASN	N-CA-C	-6.35	104.43	111.36
1	A	745	SER	N-CA-C	-6.32	102.15	110.43
1	A	497	ASP	N-CA-C	-6.27	98.68	108.90
1	B	584	SER	N-CA-C	6.27	119.43	109.65
1	B	204	GLU	N-CA-C	6.25	121.18	113.50
1	B	231	VAL	CA-C-N	6.22	127.08	120.11
1	B	231	VAL	C-N-CA	6.22	127.08	120.11
1	B	745	SER	N-CA-C	-6.19	102.33	110.43
1	A	146	ILE	CA-C-N	6.17	127.55	119.84
1	A	146	ILE	C-N-CA	6.17	127.55	119.84
1	B	210	SER	N-CA-C	6.17	119.17	110.23
1	A	459	SER	N-CA-C	-6.14	99.89	109.72
1	B	156	SER	N-CA-C	-6.12	101.90	110.35
1	A	337	CYS	CA-C-N	6.09	126.44	119.93
1	A	337	CYS	C-N-CA	6.09	126.44	119.93
1	A	584	SER	N-CA-C	5.91	118.88	109.65
1	A	231	VAL	CA-C-N	5.89	126.70	120.11
1	A	231	VAL	C-N-CA	5.89	126.70	120.11
1	A	156	SER	N-CA-C	-5.88	102.24	110.35
1	A	175	GLU	CA-C-N	5.80	127.09	119.84
1	A	175	GLU	C-N-CA	5.80	127.09	119.84
1	A	657	VAL	N-CA-C	-5.75	100.12	108.17
1	A	210	SER	N-CA-C	5.72	118.53	110.23
1	A	344	ILE	N-CA-C	5.68	116.12	108.17
1	A	272	ASP	N-CA-C	5.66	118.22	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	CYS	CA-C-N	5.64	125.97	119.93
1	B	337	CYS	C-N-CA	5.64	125.97	119.93
1	B	175	GLU	CA-C-N	5.63	126.88	119.84
1	B	175	GLU	C-N-CA	5.63	126.88	119.84
1	A	305	SER	N-CA-C	-5.55	100.41	108.07
1	A	299	CYS	N-CA-C	5.54	118.16	111.40
1	B	741	HIS	N-CA-C	-5.49	106.53	113.18
1	B	518	ILE	N-CA-C	-5.46	100.74	109.20
1	B	342	GLU	N-CA-C	5.43	117.06	111.03
1	A	199	TRP	N-CA-C	5.37	116.83	110.97
1	B	272	ASP	N-CA-C	5.36	117.87	111.71
1	B	344	ILE	N-CA-C	5.35	115.66	108.17
1	A	403	TRP	N-CA-C	-5.31	100.84	108.60
1	B	403	TRP	N-CA-C	-5.30	100.87	108.60
1	B	657	VAL	N-CA-C	-5.27	100.79	108.17
1	B	299	CYS	N-CA-C	5.27	117.83	111.40
1	B	199	TRP	N-CA-C	5.25	116.69	110.97
1	A	699	VAL	N-CA-C	5.25	115.12	107.88
1	B	305	SER	N-CA-C	-5.20	100.89	108.07
1	B	398	ILE	N-CA-C	-5.19	107.92	112.90
1	B	699	VAL	N-CA-C	5.18	115.03	107.88
1	A	518	ILE	N-CA-C	-5.17	101.20	109.17
1	A	271	THR	N-CA-C	5.16	116.90	111.28
1	A	398	ILE	N-CA-C	-5.13	107.97	112.90
1	A	744	ALA	N-CA-C	5.13	119.49	112.88
1	A	548	TYR	N-CA-C	-5.10	99.94	110.80
1	A	342	GLU	N-CA-C	5.07	116.66	111.03
1	A	631	SER	CA-C-O	-5.04	113.30	120.51
1	B	486	SER	N-CA-C	5.02	117.40	111.33

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	5920	0	5631	315	0
1	B	5920	0	5632	315	0
2	A	18	0	21	0	0
All	All	11858	0	11284	628	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (628) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:GLN:HB3	1:A:767:ARG:HB3	1.39	1.03
1:B:349:THR:HB	1:B:593:HIS:HD2	1.26	0.99
1:A:460:VAL:HG22	1:A:461:SER:H	1.28	0.99
1:A:349:THR:HB	1:A:593:HIS:HD2	1.25	0.98
1:B:761:GLN:HB3	1:B:767:ARG:HB3	1.42	0.98
1:B:52:ARG:HB2	1:B:52:ARG:HH11	1.29	0.97
1:B:624:ARG:HH11	1:B:624:ARG:HB2	1.30	0.97
1:B:386:GLN:HG3	1:B:390:LYS:NZ	1.80	0.96
1:A:624:ARG:HB2	1:A:624:ARG:HH11	1.29	0.95
1:A:518:ILE:HD13	1:A:519:VAL:H	1.33	0.94
1:A:386:GLN:HG3	1:A:390:LYS:NZ	1.83	0.94
1:A:52:ARG:HB2	1:A:52:ARG:HH11	1.29	0.94
1:B:460:VAL:HG22	1:B:461:SER:H	1.29	0.94
1:A:54:LYS:H	1:A:498:ASN:HD21	1.17	0.92
1:A:383:CYS:HB3	1:A:397:PHE:HA	1.52	0.91
1:A:91:SER:HA	1:A:94:GLU:OE1	1.71	0.91
1:B:518:ILE:HD13	1:B:519:VAL:H	1.36	0.91
1:A:349:THR:HB	1:A:593:HIS:CD2	2.07	0.90
1:B:349:THR:HB	1:B:593:HIS:CD2	2.07	0.90
1:B:383:CYS:HB3	1:B:397:PHE:HA	1.54	0.89
1:A:151:GLN:HE22	1:A:168:ASN:H	1.17	0.89
1:B:151:GLN:HE22	1:B:168:ASN:H	1.20	0.89
1:B:91:SER:HA	1:B:94:GLU:OE1	1.73	0.87
1:A:412:THR:HG22	1:A:414:ASP:H	1.37	0.87
1:A:688:THR:HG22	1:A:691:SER:H	1.40	0.87
1:B:54:LYS:H	1:B:498:ASN:HD21	1.19	0.87
1:B:688:THR:HG22	1:B:691:SER:H	1.39	0.86
1:B:690:MET:CE	1:B:720:ILE:HA	2.08	0.84
1:B:412:THR:HG22	1:B:414:ASP:H	1.41	0.83
1:A:690:MET:CE	1:A:720:ILE:HA	2.09	0.82
1:A:79:ALA:O	1:A:80:GLU:HB2	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:O	1:B:80:GLU:HB2	1.82	0.80
1:B:617:MET:HE2	1:B:619:PHE:HZ	1.48	0.79
1:B:598:ARG:HB3	1:B:683:HIS:HD2	1.47	0.79
1:A:52:ARG:HB2	1:A:52:ARG:NH1	1.96	0.79
1:B:52:ARG:HB2	1:B:52:ARG:NH1	1.97	0.79
1:A:277:THR:HG21	1:A:279:THR:O	1.84	0.78
1:A:386:GLN:HG3	1:A:390:LYS:HZ1	1.48	0.78
1:A:617:MET:HE2	1:A:619:PHE:HZ	1.48	0.78
1:A:235:GLU:OE2	1:A:251:TRP:HB3	1.84	0.78
1:B:652:ILE:HG21	1:B:756:MET:HE3	1.64	0.78
1:A:598:ARG:HB3	1:A:683:HIS:HD2	1.48	0.78
1:B:235:GLU:OE2	1:B:251:TRP:HB3	1.83	0.77
1:A:460:VAL:HG22	1:A:461:SER:N	1.99	0.77
1:B:277:THR:HG21	1:B:279:THR:O	1.85	0.77
1:B:639:MET:CE	1:B:689:VAL:HA	2.16	0.76
1:B:628:TRP:CE3	1:B:756:MET:HE1	2.20	0.76
1:A:384:GLN:HG3	1:A:398:ILE:HD11	1.66	0.76
1:A:628:TRP:CE3	1:A:756:MET:HE1	2.19	0.76
1:A:652:ILE:HG21	1:A:756:MET:HE3	1.67	0.76
1:B:384:GLN:HG3	1:B:398:ILE:HD11	1.66	0.76
1:B:483:LEU:HB3	1:B:495:LEU:HD11	1.68	0.75
1:B:235:GLU:HG2	1:B:251:TRP:HB3	1.67	0.75
1:A:235:GLU:HG2	1:A:251:TRP:HB3	1.66	0.75
1:A:639:MET:CE	1:A:689:VAL:HA	2.15	0.75
1:B:460:VAL:HG22	1:B:461:SER:N	2.01	0.75
1:A:518:ILE:HD13	1:A:519:VAL:N	2.02	0.74
1:A:121:GLN:O	1:A:125:SER:HB2	1.88	0.74
1:B:449:ASP:O	1:B:452:PRO:HD3	1.88	0.74
1:B:624:ARG:HB2	1:B:624:ARG:NH1	2.03	0.73
1:A:612:ARG:HG3	1:A:612:ARG:HH11	1.54	0.73
1:B:52:ARG:HH11	1:B:52:ARG:CB	2.02	0.73
1:A:624:ARG:HB2	1:A:624:ARG:NH1	2.04	0.72
1:B:612:ARG:HG3	1:B:612:ARG:HH11	1.54	0.72
1:A:52:ARG:HH11	1:A:52:ARG:CB	2.01	0.72
1:A:483:LEU:HB3	1:A:495:LEU:HD11	1.70	0.72
1:A:449:ASP:O	1:A:452:PRO:HD3	1.89	0.72
1:B:121:GLN:O	1:B:125:SER:HB2	1.90	0.72
1:B:485:ARG:O	1:B:485:ARG:HG3	1.89	0.72
1:B:151:GLN:HE21	1:B:167:LYS:H	1.38	0.72
1:B:688:THR:CG2	1:B:690:MET:HG2	2.19	0.72
1:A:101:SER:HB3	1:A:115:GLU:HG2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:TYR:N	1:A:586:TYR:CD1	2.57	0.71
1:B:386:GLN:HG3	1:B:390:LYS:HZ2	1.55	0.71
1:A:80:GLU:H	1:A:493:ARG:HH22	1.38	0.71
1:B:767:ARG:HD2	1:B:767:ARG:C	2.16	0.71
1:A:151:GLN:HE21	1:A:167:LYS:H	1.39	0.71
1:A:485:ARG:O	1:A:485:ARG:HG3	1.90	0.70
1:B:529:MET:HE1	1:B:619:PHE:HE1	1.57	0.70
1:A:54:LYS:H	1:A:498:ASN:ND2	1.89	0.70
1:A:529:MET:HE1	1:A:619:PHE:HE1	1.56	0.70
1:B:403:TRP:CE3	1:B:422:GLU:HB2	2.27	0.69
1:A:688:THR:CG2	1:A:690:MET:HG2	2.21	0.69
1:B:386:GLN:HG3	1:B:390:LYS:HZ1	1.55	0.69
1:B:518:ILE:HD13	1:B:519:VAL:N	2.06	0.68
1:A:658:SER:H	1:A:716:GLN:NE2	1.91	0.68
1:A:108:ASP:OD2	1:A:110:LEU:HD12	1.93	0.68
1:A:439:ASP:OD1	1:A:441:THR:HB	1.93	0.68
1:B:54:LYS:H	1:B:498:ASN:ND2	1.90	0.68
1:B:108:ASP:OD2	1:B:110:LEU:HD12	1.93	0.68
1:B:80:GLU:H	1:B:493:ARG:HH22	1.41	0.68
1:A:107:PRO:HG2	1:A:158:GLU:O	1.94	0.68
1:B:101:SER:HB3	1:B:115:GLU:HG2	1.74	0.68
1:B:439:ASP:OD1	1:B:441:THR:HB	1.95	0.67
1:B:317:ILE:HG22	1:B:319:ASN:HB2	1.76	0.67
1:B:462:LEU:N	1:B:462:LEU:HD12	2.08	0.67
1:B:586:TYR:N	1:B:586:TYR:CD1	2.59	0.67
1:B:767:ARG:HG3	1:B:767:ARG:HH11	1.59	0.67
1:A:317:ILE:HG22	1:A:319:ASN:HB2	1.77	0.67
1:B:151:GLN:NE2	1:B:168:ASN:H	1.93	0.67
1:A:641:LEU:HD11	1:A:651:GLY:HA3	1.77	0.66
1:B:617:MET:HE2	1:B:619:PHE:CZ	2.30	0.66
1:B:639:MET:HE3	1:B:689:VAL:HA	1.77	0.66
1:B:107:PRO:HG2	1:B:158:GLU:O	1.95	0.66
1:A:403:TRP:CE3	1:A:422:GLU:HB2	2.30	0.66
1:A:767:ARG:HG3	1:A:767:ARG:HH11	1.60	0.66
1:A:151:GLN:NE2	1:A:167:LYS:N	2.44	0.66
1:B:78:ASN:HB3	1:B:83:ASN:HB3	1.77	0.66
1:A:462:LEU:HD12	1:A:462:LEU:N	2.10	0.65
1:A:54:LYS:N	1:A:498:ASN:HD21	1.92	0.65
1:B:151:GLN:NE2	1:B:167:LYS:N	2.43	0.65
1:B:688:THR:HG23	1:B:690:MET:HG2	1.77	0.65
1:A:151:GLN:HE22	1:A:168:ASN:N	1.92	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:HIS:CD2	1:A:399:THR:HG22	2.30	0.65
1:A:690:MET:HE1	1:A:720:ILE:HA	1.79	0.65
1:B:151:GLN:HE22	1:B:168:ASN:N	1.94	0.65
1:B:598:ARG:HB3	1:B:683:HIS:CD2	2.31	0.65
1:B:454:ARG:NH1	1:B:480:LEU:HB2	2.12	0.65
1:A:235:GLU:CG	1:A:251:TRP:HB3	2.26	0.65
1:B:54:LYS:N	1:B:498:ASN:HD21	1.93	0.65
1:B:412:THR:HG22	1:B:413:SER:N	2.11	0.65
1:B:658:SER:H	1:B:716:GLN:NE2	1.94	0.65
1:B:690:MET:HE1	1:B:720:ILE:HA	1.79	0.64
1:A:598:ARG:HB3	1:A:683:HIS:CD2	2.33	0.64
1:A:130:TYR:HB2	1:A:146:ILE:HD13	1.80	0.64
1:A:267:PHE:CE2	1:A:284:GLN:HB2	2.33	0.64
1:A:639:MET:HE3	1:A:689:VAL:HA	1.80	0.64
1:B:235:GLU:CG	1:B:251:TRP:HB3	2.28	0.64
1:A:767:ARG:C	1:A:767:ARG:HD2	2.22	0.64
1:B:641:LEU:HD11	1:B:651:GLY:HA3	1.80	0.64
1:A:216:PRO:O	1:A:306:GLU:HG3	1.98	0.64
1:B:81:HIS:O	1:B:83:ASN:N	2.30	0.64
1:B:412:THR:CG2	1:B:413:SER:N	2.61	0.64
1:A:688:THR:HG23	1:A:690:MET:HG2	1.80	0.63
1:A:392:GLU:C	1:A:393:GLN:HG3	2.23	0.63
1:A:617:MET:HE2	1:A:619:PHE:CZ	2.31	0.63
1:A:81:HIS:O	1:A:83:ASN:N	2.32	0.63
1:B:89:GLU:C	1:B:91:SER:N	2.51	0.63
1:A:641:LEU:HD22	1:A:699:VAL:HG11	1.79	0.63
1:A:151:GLN:NE2	1:A:168:ASN:H	1.93	0.62
1:A:690:MET:HE2	1:A:719:GLN:O	1.98	0.62
1:B:267:PHE:CE2	1:B:284:GLN:HB2	2.33	0.62
1:A:78:ASN:HB3	1:A:83:ASN:HB3	1.79	0.62
1:A:595:ILE:CG2	1:A:599:LEU:HD23	2.30	0.62
1:A:89:GLU:C	1:A:91:SER:N	2.50	0.62
1:A:412:THR:HG22	1:A:413:SER:N	2.13	0.62
1:B:392:GLU:C	1:B:393:GLN:HG3	2.24	0.62
1:B:265:LYS:HG2	1:B:284:GLN:HE22	1.64	0.62
1:A:601:THR:HG22	1:A:602:LEU:N	2.15	0.62
1:B:601:THR:HG22	1:B:602:LEU:N	2.14	0.61
1:A:412:THR:CG2	1:A:413:SER:N	2.62	0.61
1:B:216:PRO:O	1:B:306:GLU:HG3	2.00	0.61
1:A:454:ARG:NH1	1:A:480:LEU:HB2	2.15	0.61
1:B:690:MET:HE2	1:B:719:GLN:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:ILE:HG23	1:B:416:LEU:HD11	1.83	0.61
1:A:235:GLU:CD	1:A:251:TRP:HB3	2.26	0.61
1:A:332:THR:O	1:A:334:VAL:HG23	2.01	0.61
1:B:116:TYR:O	1:B:117:ASN:HB2	2.00	0.61
1:B:146:ILE:HD12	1:B:153:ILE:HD12	1.83	0.61
1:B:151:GLN:HE21	1:B:167:LYS:N	1.99	0.61
1:A:460:VAL:CG2	1:A:461:SER:H	2.08	0.60
1:A:323:MET:O	1:A:342:GLU:O	2.20	0.60
1:B:460:VAL:CG2	1:B:461:SER:H	2.09	0.60
1:A:662:TYR:OH	1:A:719:GLN:HG2	2.01	0.60
1:B:401:GLY:HA3	1:B:403:TRP:NE1	2.16	0.60
1:B:508:VAL:CG1	1:B:510:MET:HE3	2.32	0.60
1:A:235:GLU:HG2	1:A:251:TRP:CB	2.32	0.60
1:B:235:GLU:CD	1:B:251:TRP:HB3	2.27	0.60
1:A:151:GLN:NE2	1:A:167:LYS:H	2.00	0.59
1:B:67:LEU:HD22	1:B:74:ILE:HG22	1.83	0.59
1:A:713:HIS:O	1:A:714:PHE:HB3	2.01	0.59
1:A:277:THR:CG2	1:A:279:THR:O	2.51	0.59
1:B:595:ILE:CG2	1:B:599:LEU:HD23	2.31	0.59
1:A:447:SER:HB2	1:A:458:TYR:CE1	2.36	0.59
1:A:265:LYS:HG2	1:A:284:GLN:HE22	1.67	0.59
1:B:447:SER:HB2	1:B:458:TYR:CE1	2.38	0.59
1:A:91:SER:O	1:A:93:PHE:N	2.35	0.59
1:A:508:VAL:CG1	1:A:510:MET:HE3	2.31	0.59
1:B:41:TYR:HB2	1:B:510:MET:HE1	1.85	0.59
1:A:125:SER:O	1:A:126:TYR:HB3	2.02	0.59
1:B:235:GLU:HG2	1:B:251:TRP:CB	2.33	0.59
1:B:332:THR:O	1:B:334:VAL:HG23	2.03	0.59
1:A:408:ILE:HG23	1:A:416:LEU:HD11	1.85	0.59
1:B:91:SER:O	1:B:93:PHE:N	2.35	0.59
1:B:652:ILE:CG2	1:B:756:MET:HE3	2.33	0.59
1:B:690:MET:HE1	1:B:720:ILE:CA	2.33	0.59
1:A:151:GLN:HE21	1:A:167:LYS:N	2.00	0.58
1:B:697:LYS:HG2	1:B:729:VAL:HG22	1.85	0.58
1:A:297:TYR:CE2	1:A:666:VAL:HG22	2.39	0.58
1:B:612:ARG:HG3	1:B:612:ARG:NH1	2.19	0.58
1:A:639:MET:HE1	1:A:688:THR:O	2.03	0.58
1:B:151:GLN:NE2	1:B:167:LYS:H	1.99	0.58
1:A:41:TYR:HB2	1:A:510:MET:HE1	1.85	0.58
1:B:381:HIS:CD2	1:B:399:THR:HG22	2.38	0.58
1:B:510:MET:HA	1:B:510:MET:HE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LYS:NZ	1:B:713:HIS:HD2	2.02	0.57
1:A:547:VAL:HG12	1:A:548:TYR:N	2.19	0.57
1:A:146:ILE:HD12	1:A:153:ILE:HD12	1.86	0.57
1:A:547:VAL:HG21	1:A:627:ILE:HD11	1.86	0.57
1:A:612:ARG:HG3	1:A:612:ARG:NH1	2.19	0.57
1:B:81:HIS:C	1:B:83:ASN:H	2.13	0.57
1:B:545:ILE:HG22	1:B:547:VAL:HG22	1.86	0.57
1:A:690:MET:HE1	1:A:720:ILE:CA	2.34	0.57
1:B:55:SER:HA	1:B:481:TYR:CE1	2.38	0.57
1:B:297:TYR:CE2	1:B:666:VAL:HG22	2.40	0.57
1:B:488:ASP:O	1:B:489:GLN:HB2	2.05	0.57
1:B:742:GLY:O	1:B:743:ILE:C	2.46	0.57
1:B:511:PRO:HD3	1:B:570:SER:HB2	1.87	0.57
1:A:116:TYR:O	1:A:117:ASN:HB2	2.05	0.56
1:B:713:HIS:O	1:B:714:PHE:HB3	2.04	0.56
1:A:67:LEU:HD22	1:A:74:ILE:HG22	1.86	0.56
1:B:146:ILE:CD1	1:B:153:ILE:HD12	2.36	0.56
1:B:256:LYS:HZ3	1:B:713:HIS:HD2	1.51	0.56
1:B:323:MET:O	1:B:342:GLU:O	2.24	0.56
1:B:641:LEU:HD22	1:B:699:VAL:HG11	1.85	0.56
1:B:662:TYR:OH	1:B:719:GLN:HG2	2.04	0.56
1:A:697:LYS:HG2	1:A:729:VAL:HG22	1.87	0.56
1:B:125:SER:O	1:B:126:TYR:HB3	2.05	0.56
1:B:158:GLU:HG2	1:B:217:ASN:HA	1.87	0.56
1:A:158:GLU:HG2	1:A:217:ASN:HA	1.88	0.56
1:A:401:GLY:HA3	1:A:403:TRP:NE1	2.21	0.56
1:A:510:MET:HE2	1:A:510:MET:HA	1.87	0.56
1:A:89:GLU:HB2	1:A:91:SER:HB3	1.88	0.56
1:A:256:LYS:NZ	1:A:713:HIS:HD2	2.03	0.56
1:A:381:HIS:CD2	1:A:399:THR:CG2	2.89	0.56
1:A:386:GLN:HG3	1:A:390:LYS:HZ2	1.68	0.56
1:A:639:MET:HE3	1:A:689:VAL:CG2	2.36	0.55
1:B:339:THR:O	1:B:342:GLU:HB2	2.06	0.55
1:B:547:VAL:HG21	1:B:627:ILE:HD11	1.88	0.55
1:A:55:SER:HA	1:A:481:TYR:CE1	2.42	0.55
1:A:256:LYS:HZ3	1:A:713:HIS:HD2	1.54	0.55
1:A:761:GLN:HB3	1:A:767:ARG:CB	2.26	0.55
1:A:370:TYR:CE2	1:A:384:GLN:HG2	2.41	0.55
1:B:401:GLY:HA3	1:B:403:TRP:HE1	1.72	0.55
1:B:639:MET:HE1	1:B:688:THR:O	2.07	0.55
1:B:767:ARG:HG3	1:B:767:ARG:NH1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLN:HG2	1:A:71:GLU:HG3	1.87	0.55
1:B:277:THR:CG2	1:B:279:THR:O	2.53	0.55
1:B:547:VAL:HG12	1:B:548:TYR:N	2.21	0.55
1:B:595:ILE:HD11	1:B:603:GLU:HB3	1.87	0.55
1:B:767:ARG:C	1:B:767:ARG:CD	2.79	0.55
1:A:339:THR:O	1:A:342:GLU:HB2	2.05	0.55
1:A:548:TYR:CD2	1:A:553:SER:HB2	2.42	0.55
1:B:707:THR:CG2	1:B:738:ASP:H	2.19	0.55
1:A:473:CYS:O	1:A:479:PRO:HA	2.07	0.55
1:B:548:TYR:CD2	1:B:553:SER:HB2	2.42	0.55
1:A:235:GLU:HG2	1:A:251:TRP:HA	1.89	0.54
1:B:235:GLU:HG2	1:B:251:TRP:HA	1.89	0.54
1:B:498:ASN:HB3	1:B:501:LEU:HB3	1.89	0.54
1:A:707:THR:CG2	1:A:738:ASP:H	2.19	0.54
1:A:511:PRO:HD3	1:A:570:SER:HB2	1.88	0.54
1:B:79:ALA:O	1:B:80:GLU:CB	2.55	0.54
1:A:299:CYS:SG	1:A:314:LEU:HD22	2.48	0.54
1:A:652:ILE:CG2	1:A:756:MET:HE3	2.36	0.54
1:B:130:TYR:HB2	1:B:146:ILE:HD13	1.89	0.54
1:B:473:CYS:O	1:B:479:PRO:HA	2.07	0.54
1:A:81:HIS:C	1:A:83:ASN:H	2.16	0.54
1:B:91:SER:CA	1:B:94:GLU:OE1	2.51	0.54
1:B:383:CYS:CB	1:B:397:PHE:HA	2.34	0.54
1:A:488:ASP:O	1:A:489:GLN:HB2	2.08	0.54
1:B:264:VAL:HG12	1:B:265:LYS:H	1.72	0.54
1:B:639:MET:HE3	1:B:689:VAL:CG2	2.38	0.54
1:A:498:ASN:HB3	1:A:501:LEU:HB3	1.90	0.54
1:B:766:LEU:O	1:B:767:ARG:O	2.26	0.54
1:A:383:CYS:CB	1:A:397:PHE:HA	2.33	0.54
1:A:767:ARG:HG3	1:A:767:ARG:NH1	2.23	0.54
1:B:205:ILE:CD1	1:B:666:VAL:HG11	2.38	0.54
1:A:690:MET:HB3	1:A:723:ALA:HB2	1.90	0.54
1:A:264:VAL:HG12	1:A:265:LYS:H	1.73	0.53
1:B:358:ALA:O	1:B:371:LYS:HE3	2.08	0.53
1:A:485:ARG:NH2	1:A:490:LYS:HD3	2.23	0.53
1:A:545:ILE:HG22	1:A:547:VAL:HG22	1.89	0.53
1:B:89:GLU:HB2	1:B:91:SER:HB3	1.89	0.53
1:B:482:THR:HG22	1:B:494:VAL:HG22	1.89	0.53
1:A:299:CYS:SG	1:A:357:PRO:HD2	2.48	0.53
1:A:595:ILE:HD11	1:A:603:GLU:HB3	1.90	0.53
1:A:205:ILE:CD1	1:A:666:VAL:HG11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:TYR:HD2	1:A:436:GLN:HA	1.73	0.53
1:A:328:TYR:HB2	1:A:335:TRP:CH2	2.44	0.53
1:A:147:PRO:HG3	1:A:164:TYR:CE1	2.44	0.53
1:A:219:THR:O	1:A:271:THR:HB	2.08	0.53
1:A:761:GLN:CB	1:A:767:ARG:HB3	2.24	0.53
1:B:70:GLN:O	1:B:73:ASN:HB2	2.09	0.53
1:B:147:PRO:HG3	1:B:164:TYR:CE1	2.45	0.53
1:B:65:GLU:HB3	1:B:76:LEU:HD11	1.90	0.52
1:A:455:CYS:HA	1:A:475:GLY:HA3	1.91	0.52
1:A:742:GLY:O	1:A:743:ILE:C	2.51	0.52
1:B:189:GLU:O	1:B:191:VAL:HG23	2.10	0.52
1:B:415:TYR:HD2	1:B:436:GLN:HA	1.74	0.52
1:B:454:ARG:HH11	1:B:480:LEU:HB2	1.75	0.52
1:B:70:GLN:HG2	1:B:71:GLU:HG3	1.90	0.52
1:B:289:ALA:C	1:B:291:VAL:H	2.17	0.52
1:B:485:ARG:NH2	1:B:490:LYS:HD3	2.24	0.52
1:A:65:GLU:HB3	1:A:76:LEU:HD11	1.91	0.52
1:A:195:GLY:C	1:A:211:ALA:HB3	2.35	0.52
1:A:583:GLY:HA2	1:A:592:MET:O	2.09	0.52
1:A:79:ALA:O	1:A:80:GLU:CB	2.55	0.52
1:A:524:ARG:HG2	1:A:524:ARG:HH11	1.74	0.52
1:B:299:CYS:SG	1:B:314:LEU:HD22	2.50	0.52
1:B:752:ILE:O	1:B:756:MET:HG3	2.10	0.52
1:B:524:ARG:HG2	1:B:524:ARG:HH11	1.74	0.51
1:B:680:ASN:HD21	1:B:683:HIS:CG	2.28	0.51
1:A:289:ALA:C	1:A:291:VAL:H	2.18	0.51
1:A:358:ALA:O	1:A:371:LYS:HE3	2.11	0.51
1:A:752:ILE:O	1:A:756:MET:HG3	2.10	0.51
1:A:766:LEU:O	1:A:767:ARG:O	2.28	0.51
1:B:398:ILE:HG22	1:B:398:ILE:O	2.10	0.51
1:B:761:GLN:CB	1:B:767:ARG:HB3	2.27	0.51
1:B:219:THR:O	1:B:271:THR:HB	2.09	0.51
1:B:81:HIS:C	1:B:83:ASN:N	2.68	0.51
1:B:229:THR:HG22	1:B:230:GLY:N	2.25	0.51
1:A:403:TRP:CD2	1:A:422:GLU:HB2	2.46	0.51
1:B:548:TYR:CE2	1:B:553:SER:HB2	2.45	0.51
1:A:320:TYR:CE2	1:A:322:VAL:HG23	2.45	0.51
1:B:195:GLY:C	1:B:211:ALA:HB3	2.35	0.51
1:B:205:ILE:HD13	1:B:666:VAL:HG11	1.92	0.51
1:B:328:TYR:HB2	1:B:335:TRP:CH2	2.45	0.51
1:A:91:SER:CA	1:A:94:GLU:OE1	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:THR:HG22	1:A:230:GLY:N	2.24	0.51
1:A:82:GLY:O	1:A:83:ASN:C	2.53	0.51
1:B:320:TYR:CE2	1:B:322:VAL:HG23	2.46	0.51
1:B:370:TYR:CE2	1:B:384:GLN:HG2	2.46	0.51
1:B:690:MET:HE1	1:B:720:ILE:CG1	2.41	0.51
1:B:84:SER:O	1:B:85:SER:HB2	2.11	0.50
1:B:299:CYS:SG	1:B:357:PRO:HD2	2.51	0.50
1:B:403:TRP:CD2	1:B:422:GLU:HB2	2.46	0.50
1:B:639:MET:O	1:B:692:ARG:NH1	2.44	0.50
1:A:680:ASN:HD21	1:A:683:HIS:CG	2.30	0.50
1:A:548:TYR:CE2	1:A:553:SER:HB2	2.46	0.50
1:B:543:LEU:HD12	1:B:575:ILE:O	2.12	0.50
1:B:75:LEU:HB2	1:B:77:PHE:HE1	1.76	0.50
1:A:129:SER:HB3	1:A:148:ASN:ND2	2.26	0.50
1:A:456:GLN:OE1	1:A:476:PRO:HG2	2.12	0.50
1:B:147:PRO:HG3	1:B:164:TYR:HE1	1.76	0.50
1:B:82:GLY:O	1:B:83:ASN:C	2.54	0.49
1:B:381:HIS:CD2	1:B:399:THR:CG2	2.95	0.49
1:B:690:MET:HB3	1:B:723:ALA:HB2	1.92	0.49
1:A:713:HIS:O	1:A:714:PHE:CB	2.61	0.49
1:B:412:THR:CG2	1:B:413:SER:H	2.25	0.49
1:B:583:GLY:HA2	1:B:592:MET:O	2.12	0.49
1:A:205:ILE:HD13	1:A:666:VAL:HG11	1.93	0.49
1:B:601:THR:HG22	1:B:602:LEU:H	1.77	0.49
1:A:398:ILE:HG22	1:A:398:ILE:O	2.12	0.49
1:A:401:GLY:HA3	1:A:403:TRP:HE1	1.78	0.49
1:A:109:ARG:O	1:A:135:LEU:HD12	2.13	0.49
1:A:375:ASP:HA	1:A:397:PHE:CZ	2.47	0.49
1:B:41:TYR:CD2	1:B:566:THR:HG22	2.47	0.49
1:B:455:CYS:HA	1:B:475:GLY:HA3	1.93	0.49
1:B:456:GLN:OE1	1:B:476:PRO:HG2	2.12	0.49
1:B:571:THR:HG22	1:B:571:THR:O	2.12	0.49
1:A:147:PRO:HG3	1:A:164:TYR:HE1	1.76	0.49
1:A:70:GLN:O	1:A:73:ASN:HB2	2.12	0.49
1:A:381:HIS:CG	1:A:399:THR:HG22	2.48	0.49
1:A:412:THR:CG2	1:A:413:SER:H	2.25	0.49
1:A:473:CYS:HB3	1:A:480:LEU:O	2.12	0.49
1:A:690:MET:HE1	1:A:720:ILE:CG1	2.43	0.49
1:B:761:GLN:HB3	1:B:767:ARG:CB	2.28	0.48
1:A:146:ILE:CD1	1:A:153:ILE:HD12	2.43	0.48
1:A:482:THR:HG22	1:A:494:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ARG:HH11	1:A:624:ARG:CB	2.14	0.48
1:B:174:ILE:HD12	1:B:174:ILE:N	2.28	0.48
1:B:713:HIS:C	1:B:715:GLN:H	2.21	0.48
1:A:41:TYR:CD2	1:A:566:THR:HG22	2.48	0.48
1:A:84:SER:O	1:A:85:SER:HB2	2.12	0.48
1:A:174:ILE:N	1:A:174:ILE:HD12	2.28	0.48
1:A:334:VAL:HG12	1:A:335:TRP:N	2.28	0.48
1:A:690:MET:HB3	1:A:723:ALA:CB	2.44	0.48
1:A:81:HIS:C	1:A:83:ASN:N	2.70	0.48
1:A:318:GLN:OE1	1:A:670:ARG:HD3	2.13	0.48
1:A:631:SER:HA	1:A:655:ALA:O	2.14	0.48
1:B:75:LEU:HB2	1:B:77:PHE:CE1	2.49	0.48
1:A:102:ASP:OD1	1:A:103:TYR:N	2.40	0.48
1:A:485:ARG:HG2	1:A:490:LYS:HB3	1.96	0.48
1:A:767:ARG:C	1:A:767:ARG:CD	2.87	0.48
1:B:109:ARG:O	1:B:135:LEU:HD12	2.13	0.48
1:B:113:LEU:HD23	1:B:132:ILE:HD13	1.95	0.48
1:A:228:ASP:OD1	1:A:262:PRO:HB3	2.14	0.48
1:A:233:LEU:HD23	1:A:253:PRO:HA	1.96	0.48
1:B:386:GLN:O	1:B:387:LYS:C	2.57	0.48
1:A:595:ILE:HG21	1:A:599:LEU:HD23	1.95	0.48
1:B:714:PHE:C	1:B:716:GLN:N	2.69	0.48
1:A:189:GLU:O	1:A:191:VAL:HG23	2.14	0.47
1:A:331:THR:HG22	1:A:332:THR:N	2.28	0.47
1:A:386:GLN:O	1:A:387:LYS:C	2.57	0.47
1:B:331:THR:HG22	1:B:332:THR:N	2.27	0.47
1:B:363:THR:HG23	1:B:368:SER:O	2.14	0.47
1:A:317:ILE:C	1:A:319:ASN:H	2.21	0.47
1:A:543:LEU:HD12	1:A:575:ILE:O	2.14	0.47
1:B:329:ASP:OD1	1:B:332:THR:N	2.47	0.47
1:A:639:MET:O	1:A:692:ARG:NH1	2.48	0.47
1:B:334:VAL:HG12	1:B:335:TRP:N	2.29	0.47
1:A:601:THR:HG22	1:A:602:LEU:H	1.78	0.47
1:A:658:SER:H	1:A:716:GLN:HE21	1.60	0.47
1:B:102:ASP:OD1	1:B:103:TYR:N	2.43	0.47
1:B:473:CYS:HB3	1:B:480:LEU:O	2.15	0.47
1:A:297:TYR:CE1	1:A:316:ARG:HA	2.50	0.47
1:A:713:HIS:C	1:A:715:GLN:H	2.22	0.47
1:B:462:LEU:N	1:B:462:LEU:CD1	2.76	0.47
1:A:163:ALA:HB2	1:A:214:TRP:CZ2	2.49	0.47
1:B:89:GLU:O	1:B:90:ASN:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:TYR:CE1	1:B:316:ARG:HA	2.50	0.47
1:B:328:TYR:HB2	1:B:335:TRP:CZ3	2.50	0.47
1:A:89:GLU:O	1:A:90:ASN:C	2.58	0.47
1:A:299:CYS:SG	1:A:314:LEU:HB2	2.55	0.47
1:A:328:TYR:HB2	1:A:335:TRP:CZ3	2.50	0.47
1:B:163:ALA:HB2	1:B:214:TRP:CZ2	2.50	0.46
1:A:363:THR:HG23	1:A:368:SER:O	2.14	0.46
1:A:647:VAL:HG12	1:A:647:VAL:O	2.14	0.46
1:B:233:LEU:HD23	1:B:253:PRO:HA	1.97	0.46
1:A:75:LEU:HB2	1:A:77:PHE:HE1	1.80	0.46
1:A:342:GLU:O	1:A:343:HIS:HB2	2.15	0.46
1:B:129:SER:HB3	1:B:148:ASN:ND2	2.29	0.46
1:B:216:PRO:O	1:B:306:GLU:OE2	2.33	0.46
1:B:264:VAL:HG12	1:B:265:LYS:N	2.30	0.46
1:B:378:GLY:O	1:B:588:GLY:HA2	2.15	0.46
1:B:680:ASN:ND2	1:B:683:HIS:HB2	2.31	0.46
1:A:168:ASN:O	1:A:194:ASN:HB2	2.15	0.46
1:B:267:PHE:CD2	1:B:284:GLN:HB2	2.51	0.46
1:B:713:HIS:O	1:B:714:PHE:CB	2.63	0.46
1:A:624:ARG:NH1	1:A:624:ARG:CB	2.76	0.46
1:B:386:GLN:HG3	1:B:390:LYS:CE	2.46	0.46
1:B:690:MET:CE	1:B:720:ILE:CA	2.87	0.46
1:A:709:ASP:OD2	1:A:741:HIS:HA	2.15	0.46
1:A:462:LEU:N	1:A:462:LEU:CD1	2.77	0.46
1:A:264:VAL:HG12	1:A:265:LYS:N	2.30	0.46
1:B:299:CYS:SG	1:B:314:LEU:HB2	2.55	0.46
1:B:375:ASP:HA	1:B:397:PHE:CZ	2.50	0.46
1:A:430:ARG:HG2	1:A:457:TYR:CE1	2.51	0.45
1:A:518:ILE:CD1	1:A:519:VAL:N	2.77	0.45
1:B:168:ASN:O	1:B:194:ASN:HB2	2.16	0.45
1:B:317:ILE:C	1:B:319:ASN:H	2.24	0.45
1:A:267:PHE:CD2	1:A:284:GLN:HB2	2.50	0.45
1:A:658:SER:HB2	1:A:690:MET:SD	2.57	0.45
1:B:595:ILE:HG22	1:B:599:LEU:HD23	1.96	0.45
1:A:120:LYS:CG	1:A:121:GLN:N	2.79	0.45
1:A:182:ARG:HH21	1:A:185:SER:HA	1.81	0.45
1:A:721:SER:O	1:A:725:VAL:HG23	2.17	0.45
1:A:737:THR:HB	1:B:722:LYS:HB2	1.98	0.45
1:B:92:THR:O	1:B:95:ILE:HG13	2.17	0.45
1:B:601:THR:CG2	1:B:602:LEU:H	2.30	0.45
1:B:709:ASP:OD2	1:B:741:HIS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PRO:O	1:A:306:GLU:OE2	2.35	0.45
1:A:378:GLY:O	1:A:588:GLY:HA2	2.17	0.45
1:A:579:PHE:CD2	1:A:610:ALA:HB2	2.51	0.45
1:B:222:ALA:HB1	1:B:266:PHE:CZ	2.51	0.45
1:B:557:ASP:OD1	1:B:561:ARG:NH2	2.50	0.45
1:A:415:TYR:CD2	1:A:436:GLN:HA	2.52	0.45
1:A:655:ALA:HA	1:A:705:HIS:CE1	2.51	0.45
1:B:690:MET:HE2	1:B:719:GLN:C	2.42	0.45
1:A:148:ASN:HD22	1:A:148:ASN:HA	1.56	0.45
1:A:370:TYR:OH	1:A:384:GLN:NE2	2.50	0.45
1:B:690:MET:HB3	1:B:723:ALA:CB	2.46	0.45
1:A:383:CYS:HB2	1:A:396:THR:C	2.42	0.45
1:B:120:LYS:CG	1:B:121:GLN:N	2.79	0.45
1:B:312:GLN:HG2	1:B:323:MET:HG3	1.98	0.45
1:A:595:ILE:HG22	1:A:599:LEU:HD23	1.98	0.45
1:A:680:ASN:ND2	1:A:683:HIS:HB2	2.32	0.45
1:B:639:MET:HE3	1:B:689:VAL:CA	2.46	0.45
1:B:658:SER:HB2	1:B:690:MET:SD	2.57	0.45
1:A:312:GLN:HG2	1:A:323:MET:HG3	1.98	0.44
1:A:492:LEU:HB3	1:A:493:ARG:NH1	2.32	0.44
1:A:557:ASP:OD1	1:A:561:ARG:NH2	2.49	0.44
1:B:91:SER:OG	1:B:92:THR:N	2.49	0.44
1:B:228:ASP:OD1	1:B:262:PRO:HB3	2.17	0.44
1:B:485:ARG:HG2	1:B:490:LYS:HB3	1.99	0.44
1:B:520:LEU:O	1:B:521:ASN:C	2.59	0.44
1:B:579:PHE:CD2	1:B:610:ALA:HB2	2.52	0.44
1:B:618:GLY:O	1:B:620:VAL:N	2.47	0.44
1:A:509:GLN:O	1:A:533:PRO:HG3	2.17	0.44
1:B:318:GLN:OE1	1:B:670:ARG:HD3	2.16	0.44
1:B:506:GLN:HA	1:B:506:GLN:OE1	2.17	0.44
1:A:639:MET:HE3	1:A:689:VAL:CA	2.47	0.44
1:B:147:PRO:HB2	1:B:166:TRP:CD1	2.52	0.44
1:A:84:SER:O	1:A:85:SER:CB	2.65	0.44
1:A:383:CYS:HB2	1:A:396:THR:O	2.17	0.44
1:A:618:GLY:O	1:A:620:VAL:N	2.46	0.44
1:B:509:GLN:O	1:B:533:PRO:HG3	2.18	0.44
1:B:647:VAL:O	1:B:647:VAL:HG12	2.16	0.44
1:A:61:VAL:HG11	1:A:109:ARG:CD	2.48	0.44
1:A:113:LEU:HD23	1:A:132:ILE:HD13	2.00	0.44
1:A:235:GLU:HG2	1:A:251:TRP:CA	2.48	0.44
1:B:84:SER:O	1:B:85:SER:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLN:HG3	1:A:390:LYS:CE	2.46	0.44
1:A:529:MET:CE	1:A:575:ILE:HG21	2.47	0.44
1:A:75:LEU:HB2	1:A:77:PHE:CE1	2.52	0.44
1:A:690:MET:HE2	1:A:719:GLN:C	2.42	0.44
1:B:93:PHE:O	1:B:100:ILE:HG13	2.18	0.44
1:B:235:GLU:HG2	1:B:251:TRP:CA	2.48	0.44
1:A:93:PHE:O	1:A:100:ILE:HG13	2.18	0.44
1:A:147:PRO:HB2	1:A:166:TRP:CD1	2.53	0.44
1:A:524:ARG:HH11	1:A:524:ARG:CG	2.30	0.44
1:B:529:MET:HE3	1:B:575:ILE:HG21	1.99	0.44
1:B:532:PRO:O	1:B:533:PRO:C	2.61	0.44
1:B:595:ILE:O	1:B:596:ASN:C	2.60	0.44
1:B:53:VAL:HG22	1:B:501:LEU:HD22	1.99	0.43
1:B:122:TRP:CE3	1:B:122:TRP:N	2.86	0.43
1:A:506:GLN:OE1	1:A:506:GLN:HA	2.18	0.43
1:B:423:TYR:CZ	1:B:424:LYS:HE3	2.52	0.43
1:A:601:THR:CG2	1:A:602:LEU:H	2.31	0.43
1:A:125:SER:OG	1:A:202:GLU:OE1	2.35	0.43
1:A:329:ASP:OD1	1:A:332:THR:N	2.50	0.43
1:A:529:MET:HE3	1:A:575:ILE:HG21	2.00	0.43
1:A:532:PRO:O	1:A:533:PRO:C	2.60	0.43
1:A:552:CYS:HB2	1:A:592:MET:SD	2.59	0.43
1:B:158:GLU:N	1:B:158:GLU:CD	2.76	0.43
1:B:286:THR:O	1:B:287:ALA:C	2.61	0.43
1:B:492:LEU:HB3	1:B:493:ARG:NH1	2.32	0.43
1:B:659:ARG:HG2	1:B:662:TYR:CE2	2.53	0.43
1:A:89:GLU:C	1:A:91:SER:H	2.25	0.43
1:A:122:TRP:N	1:A:122:TRP:CE3	2.86	0.43
1:A:550:GLY:HA2	1:A:632:TYR:CE2	2.53	0.43
1:A:595:ILE:O	1:A:596:ASN:C	2.62	0.43
1:B:370:TYR:OH	1:B:384:GLN:NE2	2.50	0.43
1:A:120:LYS:HE3	1:A:740:ASP:OD2	2.19	0.43
1:A:605:GLU:O	1:A:608:ILE:N	2.49	0.43
1:B:157:GLN:HB2	1:B:158:GLU:OE2	2.19	0.43
1:A:690:MET:CE	1:A:720:ILE:CA	2.88	0.43
1:A:747:THR:HG21	1:B:726:ASP:HA	2.01	0.43
1:B:342:GLU:O	1:B:343:HIS:HB2	2.18	0.43
1:B:415:TYR:CD2	1:B:436:GLN:HA	2.53	0.43
1:A:92:THR:O	1:A:95:ILE:HG13	2.18	0.43
1:A:157:GLN:HB2	1:A:158:GLU:OE2	2.19	0.43
1:A:520:LEU:O	1:A:522:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:TYR:C	1:B:118:TYR:CD2	2.96	0.43
1:B:161:LYS:NZ	1:B:271:THR:HG21	2.34	0.43
1:A:118:TYR:C	1:A:118:TYR:CD2	2.96	0.43
1:A:308:ARG:HA	1:A:326:CYS:O	2.19	0.43
1:A:529:MET:HG2	1:A:577:ALA:HB2	2.00	0.43
1:A:650:CYS:HB3	1:A:700:GLU:HB2	2.00	0.43
1:B:330:LYS:O	1:B:333:LEU:HD23	2.19	0.43
1:B:529:MET:CE	1:B:575:ILE:HG21	2.48	0.43
1:A:158:GLU:CD	1:A:158:GLU:N	2.77	0.43
1:B:182:ARG:HH21	1:B:185:SER:HA	1.84	0.43
1:B:217:ASN:HB2	1:B:306:GLU:OE2	2.19	0.43
1:B:715:GLN:HE21	1:B:715:GLN:HB3	1.58	0.43
1:A:423:TYR:CZ	1:A:424:LYS:HE3	2.53	0.42
1:A:536:ASP:HB3	1:A:539:LYS:NZ	2.34	0.42
1:A:635:TYR:OH	1:A:687:SER:HB2	2.18	0.42
1:B:178:LEU:HB3	1:B:179:PRO:HD2	2.01	0.42
1:B:605:GLU:O	1:B:608:ILE:N	2.52	0.42
1:A:53:VAL:HG22	1:A:501:LEU:HD22	2.01	0.42
1:A:222:ALA:HB1	1:A:266:PHE:CZ	2.55	0.42
1:A:520:LEU:O	1:A:521:ASN:C	2.61	0.42
1:A:601:THR:CG2	1:A:602:LEU:N	2.77	0.42
1:B:583:GLY:HA3	1:B:595:ILE:HG13	2.02	0.42
1:A:412:THR:HG22	1:A:414:ASP:N	2.19	0.42
1:B:125:SER:OG	1:B:202:GLU:OE1	2.35	0.42
1:A:141:ILE:HG12	1:A:177:HIS:CE1	2.55	0.42
1:A:454:ARG:HH11	1:A:480:LEU:HB2	1.81	0.42
1:A:61:VAL:HG11	1:A:109:ARG:HD3	2.02	0.42
1:B:53:VAL:HG22	1:B:501:LEU:CD2	2.50	0.42
1:B:399:THR:HG23	1:B:403:TRP:CH2	2.55	0.42
1:B:449:ASP:O	1:B:450:LEU:C	2.62	0.42
1:B:690:MET:HE1	1:B:720:ILE:HG12	2.00	0.42
1:A:330:LYS:O	1:A:333:LEU:HD23	2.19	0.42
1:A:583:GLY:HA3	1:A:595:ILE:HG13	2.00	0.42
1:B:308:ARG:HA	1:B:326:CYS:O	2.19	0.42
1:B:650:CYS:HB3	1:B:700:GLU:HB2	2.02	0.42
1:A:521:ASN:O	1:A:522:GLU:HB2	2.20	0.42
1:A:601:THR:HG22	1:A:602:LEU:HD23	2.02	0.42
1:B:59:ARG:HB2	1:B:67:LEU:HB2	2.02	0.42
1:B:66:TYR:CE1	1:B:77:PHE:HB2	2.55	0.42
1:B:132:ILE:HG21	1:B:176:PRO:HB3	2.00	0.42
1:B:142:THR:O	1:B:145:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:ARG:HH11	1:B:524:ARG:CG	2.31	0.42
1:A:639:MET:HE3	1:A:689:VAL:HG23	2.00	0.42
1:A:714:PHE:C	1:A:716:GLN:N	2.72	0.42
1:B:383:CYS:HB2	1:B:396:THR:O	2.20	0.42
1:B:536:ASP:HB3	1:B:539:LYS:NZ	2.34	0.42
1:B:655:ALA:HA	1:B:705:HIS:CE1	2.55	0.42
1:A:655:ALA:N	1:A:656:PRO:CD	2.83	0.42
1:B:383:CYS:HB2	1:B:396:THR:C	2.45	0.42
1:B:152:TRP:CE2	1:B:210:SER:HB2	2.54	0.42
1:B:688:THR:HG22	1:B:691:SER:N	2.21	0.42
1:A:152:TRP:CE2	1:A:210:SER:HB2	2.55	0.41
1:A:571:THR:O	1:A:571:THR:HG22	2.20	0.41
1:B:75:LEU:HD23	1:B:86:ILE:HA	2.02	0.41
1:B:527:TYR:HB3	1:B:579:PHE:HD1	1.85	0.41
1:B:61:VAL:O	1:B:61:VAL:HG12	2.19	0.41
1:B:595:ILE:HG21	1:B:599:LEU:HD23	1.99	0.41
1:B:679:ASP:OD1	1:B:679:ASP:C	2.63	0.41
1:B:89:GLU:C	1:B:91:SER:H	2.26	0.41
1:B:632:TYR:O	1:B:635:TYR:HB3	2.19	0.41
1:A:532:PRO:O	1:A:533:PRO:O	2.38	0.41
1:B:61:VAL:HG11	1:B:109:ARG:CD	2.50	0.41
1:B:430:ARG:HG2	1:B:457:TYR:CE1	2.54	0.41
1:A:454:ARG:NH1	1:A:478:LEU:O	2.53	0.41
1:B:690:MET:HE1	1:B:720:ILE:N	2.36	0.41
1:A:61:VAL:O	1:A:61:VAL:HG12	2.20	0.41
1:A:132:ILE:HG21	1:A:176:PRO:HB3	2.02	0.41
1:B:552:CYS:HB2	1:B:592:MET:SD	2.61	0.41
1:A:329:ASP:OD1	1:A:329:ASP:C	2.63	0.41
1:B:166:TRP:O	1:B:167:LYS:HB2	2.21	0.41
1:B:449:ASP:O	1:B:451:ASN:N	2.54	0.41
1:B:529:MET:HG2	1:B:577:ALA:HB2	2.03	0.41
1:B:649:LYS:NZ	1:B:763:CYS:O	2.48	0.41
1:B:550:GLY:HA2	1:B:632:TYR:CE2	2.56	0.41
1:B:624:ARG:NH1	1:B:624:ARG:CB	2.78	0.41
1:B:707:THR:HG21	1:B:738:ASP:H	1.86	0.41
1:A:178:LEU:HB3	1:A:179:PRO:HD2	2.02	0.41
1:A:304:VAL:HG22	1:A:362:PHE:CD1	2.55	0.41
1:B:104:SER:HB3	1:B:113:LEU:HB2	2.02	0.41
1:B:107:PRO:C	1:B:109:ARG:H	2.29	0.41
1:B:520:LEU:O	1:B:522:GLU:N	2.54	0.41
1:B:532:PRO:O	1:B:533:PRO:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:LYS:HD3	1:B:623:LYS:HA	1.86	0.41
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.88	0.41
1:A:512:SER:OG	1:A:531:LEU:HB2	2.20	0.41
1:A:746:SER:O	1:A:750:GLN:HG3	2.21	0.41
1:A:53:VAL:HG22	1:A:501:LEU:CD2	2.50	0.40
1:A:91:SER:OG	1:A:92:THR:N	2.51	0.40
1:A:104:SER:HB3	1:A:113:LEU:HB2	2.03	0.40
1:A:513:LYS:HA	1:A:529:MET:O	2.21	0.40
1:A:690:MET:HE1	1:A:720:ILE:HG12	2.02	0.40
1:A:734:MET:HE3	1:A:755:HIS:CE1	2.56	0.40
1:A:760:LEU:HD23	1:A:760:LEU:HA	1.97	0.40
1:B:215:SER:HB3	1:B:303:TRP:CZ2	2.56	0.40
1:B:473:CYS:HB3	1:B:480:LEU:H	1.87	0.40
1:B:518:ILE:CD1	1:B:519:VAL:N	2.80	0.40
1:B:624:ARG:HH11	1:B:624:ARG:CB	2.16	0.40
1:A:246:TYR:HA	1:A:247:PRO:HD2	1.97	0.40
1:A:288:PRO:HD2	1:A:313:TRP:CD1	2.56	0.40
1:A:449:ASP:O	1:A:450:LEU:C	2.64	0.40
1:B:268:ILE:HD11	1:B:285:ILE:HD11	2.03	0.40
1:A:315:ARG:HD2	1:A:320:TYR:HB3	2.02	0.40
1:B:96:PHE:CB	1:B:100:ILE:HD11	2.52	0.40
1:B:513:LYS:HA	1:B:529:MET:O	2.22	0.40
1:B:615:LEU:HD23	1:B:620:VAL:CG1	2.51	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	728/730 (100%)	614 (84%)	87 (12%)	27 (4%)	2	15
1	B	728/730 (100%)	615 (84%)	86 (12%)	27 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1456/1460 (100%)	1229 (84%)	173 (12%)	54 (4%)	2 15

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	143	GLU
1	A	450	LEU
1	A	521	ASN
1	A	533	PRO
1	A	585	GLY
1	A	619	PHE
1	A	713	HIS
1	B	80	GLU
1	B	143	GLU
1	B	450	LEU
1	B	533	PRO
1	B	585	GLY
1	B	619	PHE
1	B	713	HIS
1	A	82	GLY
1	A	85	SER
1	A	91	SER
1	A	92	THR
1	A	318	GLN
1	A	475	GLY
1	A	534	HIS
1	B	82	GLY
1	B	85	SER
1	B	91	SER
1	B	92	THR
1	B	218	GLY
1	B	318	GLN
1	B	461	SER
1	B	475	GLY
1	B	521	ASN
1	A	147	PRO
1	A	218	GLY
1	A	391	PRO
1	A	461	SER
1	B	147	PRO
1	B	391	PRO

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Mol	Chain	Res	Type
1	B	534	HIS
1	B	596	ASN
1	A	83	ASN
1	A	290	SER
1	A	596	ASN
1	B	290	SER
1	B	740	ASP
1	A	126	TYR
1	A	274	LEU
1	A	343	HIS
1	B	83	ASN
1	B	274	LEU
1	B	343	HIS
1	A	695	ASN
1	A	740	ASP
1	B	148	ASN
1	B	766	LEU

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	643/651 (99%)	595 (92%)	48 (8%)	12	39
1	B	643/651 (99%)	596 (93%)	47 (7%)	13	40
All	All	1286/1302 (99%)	1191 (93%)	95 (7%)	13	40

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	94	GLU
1	A	122	TRP
1	A	139	GLN
1	A	146	ILE
1	A	148	ASN

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Mol	Chain	Res	Type
1	A	149	ASN
1	A	175	GLU
1	A	229	THR
1	A	260	VAL
1	A	264	VAL
1	A	277	THR
1	A	283	MET
1	A	299	CYS
1	A	300	ASP
1	A	306	GLU
1	A	340	THR
1	A	342	GLU
1	A	346	THR
1	A	349	THR
1	A	394	VAL
1	A	395	CYS
1	A	413	SER
1	A	414	ASP
1	A	441	THR
1	A	453	GLU
1	A	454	ARG
1	A	470	GLN
1	A	483	LEU
1	A	485	ARG
1	A	487	THR
1	A	504	MET
1	A	518	ILE
1	A	519	VAL
1	A	533	PRO
1	A	547	VAL
1	A	586	TYR
1	A	598	ARG
1	A	609	GLU
1	A	624	ARG
1	A	686	ASN
1	A	690	MET
1	A	698	GLN
1	A	707	THR
1	A	715	GLN
1	A	716	GLN
1	A	740	ASP
1	A	767	ARG

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Mol	Chain	Res	Type
1	B	52	ARG
1	B	94	GLU
1	B	122	TRP
1	B	139	GLN
1	B	146	ILE
1	B	148	ASN
1	B	149	ASN
1	B	175	GLU
1	B	229	THR
1	B	260	VAL
1	B	264	VAL
1	B	277	THR
1	B	283	MET
1	B	299	CYS
1	B	300	ASP
1	B	342	GLU
1	B	346	THR
1	B	349	THR
1	B	394	VAL
1	B	395	CYS
1	B	413	SER
1	B	414	ASP
1	B	441	THR
1	B	453	GLU
1	B	454	ARG
1	B	470	GLN
1	B	483	LEU
1	B	485	ARG
1	B	487	THR
1	B	504	MET
1	B	518	ILE
1	B	519	VAL
1	B	533	PRO
1	B	547	VAL
1	B	586	TYR
1	B	598	ARG
1	B	609	GLU
1	B	624	ARG
1	B	686	ASN
1	B	688	THR
1	B	690	MET
1	B	698	GLN

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Mol	Chain	Res	Type
1	B	707	THR
1	B	715	GLN
1	B	716	GLN
1	B	740	ASP
1	B	767	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	148	ASN
1	A	151	GLN
1	A	157	GLN
1	A	181	HIS
1	A	284	GLN
1	A	381	HIS
1	A	384	GLN
1	A	386	GLN
1	A	393	GLN
1	A	470	GLN
1	A	484	HIS
1	A	489	GLN
1	A	498	ASN
1	A	593	HIS
1	A	607	GLN
1	A	680	ASN
1	A	683	HIS
1	A	698	GLN
1	A	713	HIS
1	A	715	GLN
1	A	716	GLN
1	A	719	GLN
1	A	749	HIS
1	A	750	GLN
1	B	72	ASN
1	B	90	ASN
1	B	148	ASN
1	B	151	GLN
1	B	157	GLN
1	B	181	HIS
1	B	197	ASN
1	B	225	GLN

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Mol	Chain	Res	Type
1	B	284	GLN
1	B	381	HIS
1	B	384	GLN
1	B	386	GLN
1	B	470	GLN
1	B	484	HIS
1	B	489	GLN
1	B	498	ASN
1	B	593	HIS
1	B	607	GLN
1	B	680	ASN
1	B	683	HIS
1	B	698	GLN
1	B	713	HIS
1	B	715	GLN
1	B	716	GLN
1	B	719	GLN
1	B	749	HIS
1	B	750	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AIA	A	768	1	18,19,19	1.18	2 (11%)	17,26,26	1.76	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AIA	A	768	1	-	2/14/36/36	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	768	AIA	C8-N12	-2.64	1.35	1.48
2	A	768	AIA	C9-C4	2.61	1.55	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	768	AIA	C13-C9-C4	4.98	116.56	110.33
2	A	768	AIA	C7-C3-N1	2.43	104.32	101.68
2	A	768	AIA	C4-C9-N14	-2.42	106.01	110.09
2	A	768	AIA	C7-C3-C8	-2.24	103.82	112.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	768	AIA	C7-C3-C8-N12
2	A	768	AIA	N1-C3-C8-N12

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	730/730 (100%)	0.01	19 (2%) 57 36	32, 58, 91, 165	0
1	B	730/730 (100%)	0.20	25 (3%) 48 28	35, 65, 104, 161	0
All	All	1460/1460 (100%)	0.11	44 (3%) 52 31	32, 61, 99, 165	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	PHE	4.2
1	B	440	HIS	4.0
1	B	38	ARG	3.9
1	B	442	ASN	3.8
1	B	438	THR	3.7
1	B	415	TYR	3.6
1	A	158	GLU	3.6
1	B	767	ARG	3.5
1	A	767	ARG	3.5
1	A	83	ASN	3.2
1	B	444	LYS	3.2
1	B	414	ASP	3.0
1	B	158	GLU	2.9
1	B	624	ARG	2.9
1	A	96	PHE	2.8
1	A	143	GLU	2.8
1	A	40	THR	2.6
1	A	352	CYS	2.6
1	B	585	GLY	2.6
1	A	251	TRP	2.6
1	B	83	ASN	2.6
1	B	352	CYS	2.6
1	A	394	VAL	2.5
1	A	762	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	393	GLN	2.5
1	B	762	GLN	2.4
1	A	490	LYS	2.4
1	B	439	ASP	2.4
1	A	766	LEU	2.4
1	B	251	TRP	2.4
1	A	98	ASP	2.4
1	B	43	LEU	2.2
1	A	449	ASP	2.2
1	A	475	GLY	2.2
1	A	393	GLN	2.2
1	B	400	LYS	2.2
1	A	518	ILE	2.1
1	B	42	THR	2.1
1	A	319	ASN	2.1
1	B	436	GLN	2.1
1	B	69	LYS	2.0
1	A	624	ARG	2.0
1	B	40	THR	2.0
1	B	514	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AIA	A	768	18/18	0.94	0.16	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.