



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:37 AM UTC

PDB ID : 2RFW / pdb_00002rfw
Title : Crystal Structure of Cellobiohydrolase from *Melanocarpus albomyces*
Authors : Parkkinen, T.; Koivula, A.; Vehmaanper, J.; Rouvinen, J.
Deposited on : 2007-10-02
Resolution : 1.60 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

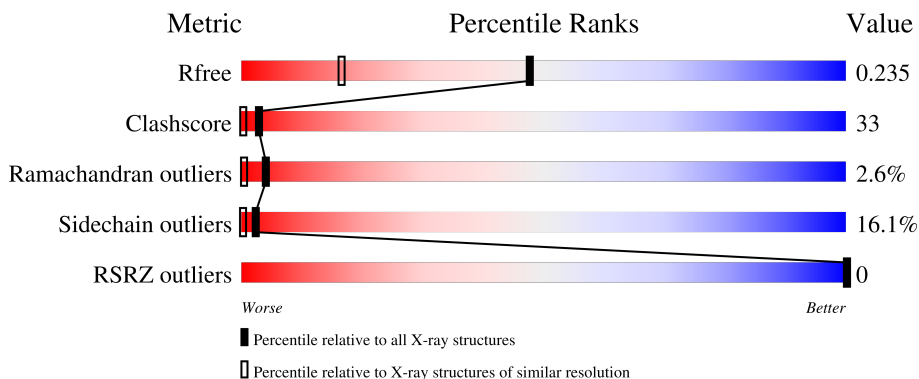
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	430	 28% 53% 16% •
1	B	430	 29% 49% 19% •
1	C	430	 54% 37% 7% •
1	D	430	 60% 32% 8% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14021 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 Cellulose 1,4-beta-cellobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	430	3333	2075	558	669	31	0	0	0
1	B	430	3333	2075	558	669	31	0	0	0
1	C	430	3333	2075	558	669	31	0	0	0
1	D	430	3333	2075	558	669	31	0	0	0

- Molecule 2 is water.

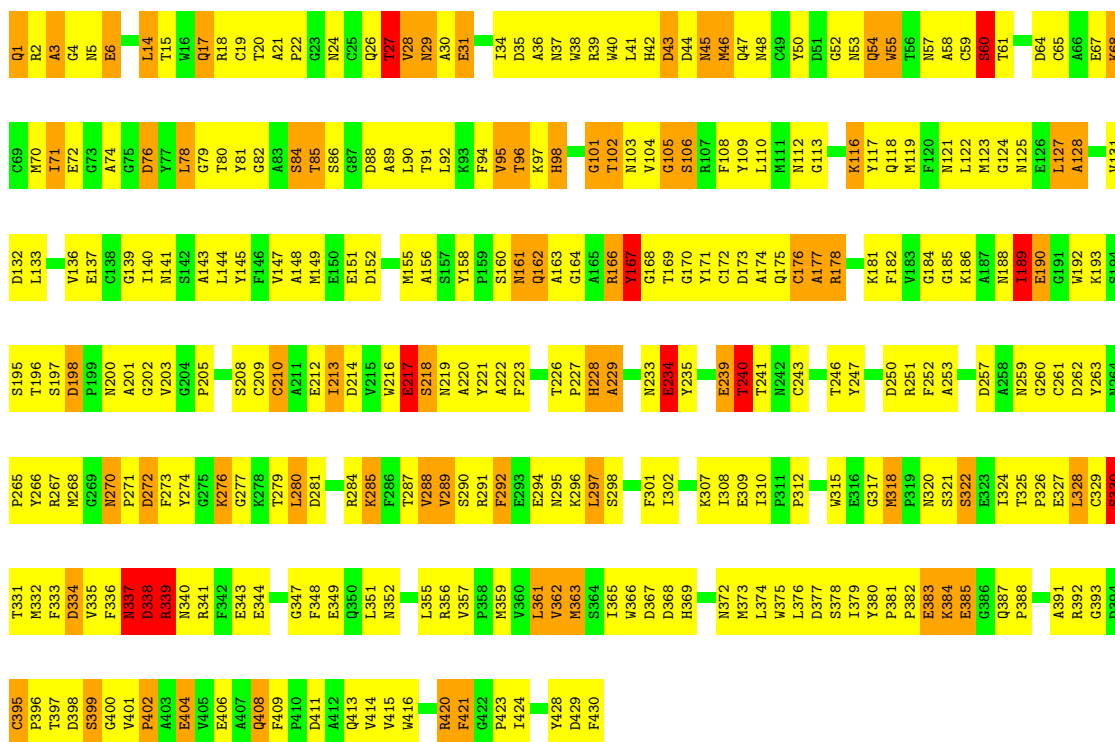
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total 139	O 139	0	0
2	B	147	Total 147	O 147	0	0
2	C	187	Total 187	O 187	0	0
2	D	216	Total 216	O 216	0	0

3 Residue-property plots

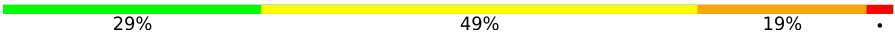
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

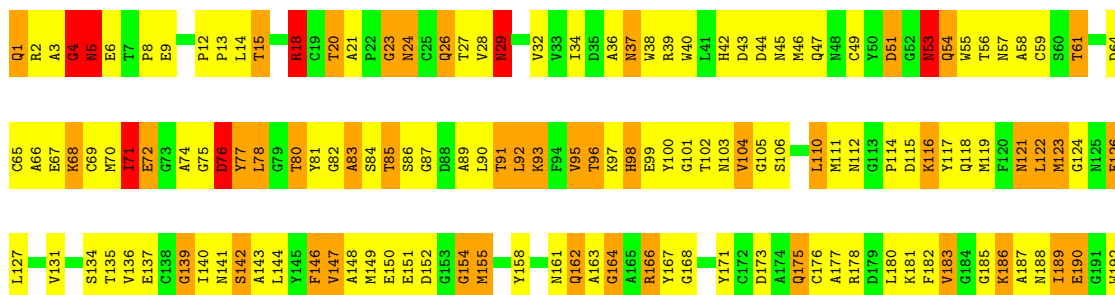
- Molecule 1: Cellulose 1,4-beta-cellobiosidase

Chain A: 



- Molecule 1: Cellulose 1,4-beta-cellobiosidase

Chain B: 



S378	I379	Y380	P381	P382	E383	K384	E385	A390	G393	D394	C395	D398	S399	G400	E406	W416	S417	N418	P423	I424	F430
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4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.94Å 94.52Å 189.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 20.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-1.60) 99.4 (20.00-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 1.60Å)	Xtrriage
Refinement program	SHELX, SHELXL-97	Depositor
R, R_{free}	0.199 , 0.243 0.199 , 0.235	Depositor DCC
R_{free} test set	11784 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	9.8	Xtrriage
Anisotropy	0.210	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.437 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14021	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.62% 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: PCA

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	0.46	0/3416	1.67	67/4648 (1.4%)
1	B	0.46	0/3416	1.68	60/4648 (1.3%)
1	C	0.53	0/3416	1.70	62/4648 (1.3%)
1	D	0.54	0/3416	1.67	62/4648 (1.3%)
All	All	0.50	0/13664	1.68	251/18592 (1.4%)

There are no bond length outliers.

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ALA	CA-C-N	17.38	146.27	121.42
1	B	148	ALA	C-N-CA	17.38	146.27	121.42
1	C	98	HIS	CA-CB-CG	11.64	125.44	113.80
1	A	382	PRO	CA-C-N	11.62	142.61	120.99
1	A	382	PRO	C-N-CA	11.62	142.61	120.99
1	B	76	ASP	CA-CB-CG	11.47	124.07	112.60
1	B	397	THR	CA-C-N	11.38	143.28	121.54
1	B	397	THR	C-N-CA	11.38	143.28	121.54
1	D	76	ASP	CA-CB-CG	11.20	123.80	112.60
1	B	98	HIS	CA-C-N	9.53	135.84	120.60
1	B	98	HIS	C-N-CA	9.53	135.84	120.60
1	C	384	LYS	CA-C-N	9.37	137.53	122.81
1	C	384	LYS	C-N-CA	9.37	137.53	122.81
1	A	228	HIS	CA-CB-CG	9.19	122.99	113.80
1	D	368	ASP	CA-CB-CG	9.18	121.78	112.60
1	A	98	HIS	CA-CB-CG	9.09	122.89	113.80
1	D	333	PHE	CA-CB-CG	-8.37	105.43	113.80
1	A	176	CYS	CA-C-N	8.32	137.43	121.54
1	A	176	CYS	C-N-CA	8.32	137.43	121.54
1	B	72	GLU	CA-C-N	8.32	131.87	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	GLU	C-N-CA	8.32	131.87	121.06
1	A	347	GLY	CA-C-N	8.22	131.97	120.29
1	A	347	GLY	C-N-CA	8.22	131.97	120.29
1	C	393	GLY	CA-C-N	-8.20	110.32	122.86
1	C	393	GLY	C-N-CA	-8.20	110.32	122.86
1	B	164	GLY	CA-C-N	8.15	131.55	120.38
1	B	164	GLY	C-N-CA	8.15	131.55	120.38
1	A	29	ASN	CA-CB-CG	-8.08	104.52	112.60
1	B	57	ASN	CA-C-N	7.96	135.01	122.60
1	B	57	ASN	C-N-CA	7.96	135.01	122.60
1	D	64	ASP	CA-CB-CG	7.92	120.52	112.60
1	D	341	ARG	CD-NE-CZ	7.76	135.27	124.40
1	A	95	VAL	CA-C-N	-7.67	112.17	122.99
1	A	95	VAL	C-N-CA	-7.67	112.17	122.99
1	D	146	PHE	CA-C-O	-7.60	112.65	120.71
1	C	120	PHE	CA-C-N	-7.39	112.52	122.72
1	C	120	PHE	C-N-CA	-7.39	112.52	122.72
1	C	16	TRP	CA-C-O	-7.38	113.54	121.36
1	D	173	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	218	SER	CA-C-N	7.21	133.57	122.11
1	A	218	SER	C-N-CA	7.21	133.57	122.11
1	B	49	CYS	CA-C-N	7.16	134.52	121.85
1	B	49	CYS	C-N-CA	7.16	134.52	121.85
1	B	4	GLY	O-C-N	-7.13	113.43	122.70
1	B	146	PHE	CA-C-N	-7.09	113.27	123.06
1	B	146	PHE	C-N-CA	-7.09	113.27	123.06
1	D	303	GLN	CA-C-O	-6.99	111.68	120.28
1	A	55	TRP	CA-C-N	6.98	134.75	122.67
1	A	55	TRP	C-N-CA	6.98	134.75	122.67
1	C	253	ALA	CB-CA-C	-6.98	102.04	111.88
1	D	115	ASP	CA-C-O	6.95	126.79	119.14
1	B	196	THR	CA-C-N	6.92	131.27	120.89
1	B	196	THR	C-N-CA	6.92	131.27	120.89
1	C	198	ASP	CA-C-N	6.89	126.52	119.56
1	C	198	ASP	C-N-CA	6.89	126.52	119.56
1	B	208	SER	CA-C-N	-6.85	110.60	123.27
1	B	208	SER	C-N-CA	-6.85	110.60	123.27
1	B	223	PHE	CA-CB-CG	6.85	120.65	113.80
1	A	260	GLY	CA-C-N	6.77	133.16	123.14
1	A	260	GLY	C-N-CA	6.77	133.16	123.14
1	A	106	SER	CA-C-N	6.75	132.29	122.77
1	A	106	SER	C-N-CA	6.75	132.29	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	GLU	CA-C-N	6.71	129.27	120.28
1	A	349	GLU	C-N-CA	6.71	129.27	120.28
1	D	66	ALA	CA-C-N	-6.70	111.48	122.54
1	D	66	ALA	C-N-CA	-6.70	111.48	122.54
1	D	252	PHE	CA-CB-CG	-6.67	107.13	113.80
1	A	421	PHE	CA-CB-CG	6.60	120.40	113.80
1	D	303	GLN	O-C-N	6.60	131.41	123.36
1	A	218	SER	N-CA-C	6.58	118.32	107.73
1	B	75	GLY	CA-C-N	6.53	131.96	122.16
1	B	75	GLY	C-N-CA	6.53	131.96	122.16
1	B	45	ASN	CA-C-N	6.50	133.96	121.54
1	B	45	ASN	C-N-CA	6.50	133.96	121.54
1	B	71	ILE	O-C-N	6.41	129.65	122.98
1	A	193	LYS	CA-C-N	6.41	130.24	120.82
1	A	193	LYS	C-N-CA	6.41	130.24	120.82
1	C	228	HIS	CA-C-O	-6.39	113.46	120.30
1	D	28	VAL	CA-C-O	-6.38	113.83	120.27
1	C	212	GLU	CA-C-N	-6.37	114.44	123.11
1	C	212	GLU	C-N-CA	-6.37	114.44	123.11
1	A	334	ASP	N-CA-C	-6.33	105.03	112.89
1	C	367	ASP	CA-CB-CG	6.32	118.92	112.60
1	C	270	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	D	394	ASP	CA-CB-CG	6.30	118.90	112.60
1	D	334	ASP	CA-CB-CG	6.29	118.89	112.60
1	C	397	THR	CA-C-N	-6.27	112.66	123.25
1	C	397	THR	C-N-CA	-6.27	112.66	123.25
1	D	114	PRO	CA-C-N	6.26	132.75	121.92
1	D	114	PRO	C-N-CA	6.26	132.75	121.92
1	C	264	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	202	GLY	CA-C-N	6.23	133.18	121.97
1	A	202	GLY	C-N-CA	6.23	133.18	121.97
1	B	154	GLY	CA-C-N	6.23	128.87	120.65
1	B	154	GLY	C-N-CA	6.23	128.87	120.65
1	C	249	GLU	CA-C-N	-6.21	114.35	123.05
1	C	249	GLU	C-N-CA	-6.21	114.35	123.05
1	A	89	ALA	N-CA-C	6.21	118.10	109.15
1	D	250	ASP	CA-C-N	6.18	129.41	120.38
1	D	250	ASP	C-N-CA	6.18	129.41	120.38
1	B	44	ASP	CA-CB-CG	6.17	118.77	112.60
1	D	393	GLY	CA-C-O	-6.17	115.61	121.60
1	C	348	PHE	CA-CB-CG	-6.01	107.79	113.80
1	C	75	GLY	CA-C-N	5.96	131.79	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	GLY	C-N-CA	5.96	131.79	122.26
1	A	28	VAL	CA-C-N	-5.95	112.67	121.24
1	A	28	VAL	C-N-CA	-5.95	112.67	121.24
1	B	236	HIS	CA-C-N	-5.92	115.86	123.19
1	B	236	HIS	C-N-CA	-5.92	115.86	123.19
1	C	205	PRO	O-C-N	5.88	128.81	122.17
1	D	111	MET	CA-C-N	5.86	132.27	123.24
1	D	111	MET	C-N-CA	5.86	132.27	123.24
1	D	377	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	395	CYS	O-C-N	5.81	127.93	121.43
1	A	3	ALA	CA-C-N	5.79	126.75	120.44
1	A	3	ALA	C-N-CA	5.79	126.75	120.44
1	A	233	ASN	CA-C-N	5.79	129.09	120.87
1	A	233	ASN	C-N-CA	5.79	129.09	120.87
1	A	338	ASP	CA-C-N	5.79	132.60	121.54
1	A	338	ASP	C-N-CA	5.79	132.60	121.54
1	A	170	GLY	N-CA-C	5.77	123.32	115.30
1	D	117	TYR	O-C-N	5.77	129.47	122.96
1	A	217	GLU	CA-C-O	-5.76	114.60	120.71
1	C	418	ASN	CA-C-N	5.76	129.19	120.77
1	C	418	ASN	C-N-CA	5.76	129.19	120.77
1	D	149	MET	CA-C-N	5.76	129.66	121.42
1	D	149	MET	C-N-CA	5.76	129.66	121.42
1	C	324	ILE	CA-C-N	5.76	132.25	123.96
1	C	324	ILE	C-N-CA	5.76	132.25	123.96
1	B	83	ALA	CA-C-N	-5.74	112.81	122.92
1	B	83	ALA	C-N-CA	-5.74	112.81	122.92
1	C	354	ALA	CA-C-O	5.74	126.51	120.42
1	D	56	THR	CA-C-N	-5.74	113.13	122.65
1	D	56	THR	C-N-CA	-5.74	113.13	122.65
1	B	18	ARG	CD-NE-CZ	5.72	132.41	124.40
1	B	255	LYS	O-C-N	5.70	129.46	122.34
1	A	128	ALA	CA-C-O	5.69	126.64	120.32
1	D	53	ASN	CA-CB-CG	5.69	118.29	112.60
1	A	229	ALA	CA-C-N	5.68	132.36	122.82
1	A	229	ALA	C-N-CA	5.68	132.36	122.82
1	D	228	HIS	CA-CB-CG	5.66	119.46	113.80
1	D	342	PHE	O-C-N	-5.65	116.25	122.07
1	C	134	SER	CA-C-N	-5.63	113.64	122.65
1	C	134	SER	C-N-CA	-5.63	113.64	122.65
1	C	39	ARG	O-C-N	5.62	130.35	123.10
1	B	53	ASN	CA-CB-CG	5.61	118.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	ASP	CA-C-N	-5.60	113.66	122.79
1	C	132	ASP	C-N-CA	-5.60	113.66	122.79
1	A	330	SER	CA-C-N	5.59	129.54	120.60
1	A	330	SER	C-N-CA	5.59	129.54	120.60
1	C	419	ILE	CA-C-O	-5.58	114.11	120.98
1	C	64	ASP	CA-CB-CG	5.58	118.18	112.60
1	D	316	GLU	O-C-N	5.58	129.73	122.87
1	D	43	ASP	CA-CB-CG	-5.56	107.04	112.60
1	B	311	PRO	CA-C-O	5.53	124.88	120.90
1	D	266	TYR	CA-CB-CG	5.53	123.86	113.90
1	A	337	ASN	CA-C-N	5.53	132.09	121.54
1	A	337	ASN	C-N-CA	5.53	132.09	121.54
1	B	139	GLY	CA-C-N	5.51	131.90	121.97
1	B	139	GLY	C-N-CA	5.51	131.90	121.97
1	B	231	THR	CA-C-N	5.50	130.41	122.44
1	B	231	THR	C-N-CA	5.50	130.41	122.44
1	B	264	ASN	CA-CB-CG	5.50	118.10	112.60
1	C	17	GLN	CA-C-N	-5.49	114.88	122.30
1	C	17	GLN	C-N-CA	-5.49	114.88	122.30
1	B	77	TYR	CA-C-N	5.49	129.05	120.82
1	B	77	TYR	C-N-CA	5.49	129.05	120.82
1	A	161	ASN	CA-CB-CG	5.47	118.07	112.60
1	D	304	ASP	CA-C-N	5.47	129.77	120.91
1	D	304	ASP	C-N-CA	5.47	129.77	120.91
1	C	409	PHE	O-C-N	-5.46	115.04	121.32
1	A	349	GLU	O-C-N	5.45	127.76	122.09
1	A	167	TYR	CA-CB-CG	5.44	123.69	113.90
1	C	377	ASP	CA-CB-CG	5.42	118.02	112.60
1	D	72	GLU	CA-C-O	5.42	128.71	121.78
1	D	221	TYR	CA-C-O	5.40	124.77	118.77
1	B	71	ILE	CB-CA-C	-5.39	102.27	110.95
1	A	101	GLY	N-CA-C	5.38	117.36	110.96
1	C	393	GLY	O-C-N	-5.38	117.43	123.61
1	C	100	TYR	CA-C-N	5.37	127.87	120.72
1	C	100	TYR	C-N-CA	5.37	127.87	120.72
1	D	416	TRP	CA-C-N	-5.37	113.06	121.87
1	D	416	TRP	C-N-CA	-5.37	113.06	121.87
1	A	334	ASP	CA-CB-CG	5.36	117.95	112.60
1	B	234	GLU	CA-C-O	-5.35	115.49	121.81
1	C	39	ARG	CA-C-N	5.35	128.70	121.05
1	C	39	ARG	C-N-CA	5.35	128.70	121.05
1	D	158	TYR	CA-C-N	5.31	124.97	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	158	TYR	C-N-CA	5.31	124.97	119.56
1	B	255	LYS	N-CA-C	-5.31	106.48	113.17
1	D	390	ALA	CA-C-N	5.30	129.89	121.99
1	D	390	ALA	C-N-CA	5.30	129.89	121.99
1	A	398	ASP	CA-C-N	5.30	131.66	121.54
1	A	398	ASP	C-N-CA	5.30	131.66	121.54
1	C	364	SER	CA-CB-OG	-5.30	100.50	111.10
1	B	5	ASN	CA-C-N	5.28	128.34	120.31
1	B	5	ASN	C-N-CA	5.28	128.34	120.31
1	C	331	THR	CA-C-N	5.28	127.66	120.54
1	C	331	THR	C-N-CA	5.28	127.66	120.54
1	B	148	ALA	O-C-N	5.27	129.34	122.38
1	A	27	THR	CA-C-N	5.26	130.26	123.10
1	A	27	THR	C-N-CA	5.26	130.26	123.10
1	A	321	SER	CA-C-N	5.26	132.82	122.61
1	A	321	SER	C-N-CA	5.26	132.82	122.61
1	B	54	GLN	CA-C-N	5.25	129.85	121.66
1	B	54	GLN	C-N-CA	5.25	129.85	121.66
1	D	270	ASN	CA-C-O	5.24	127.82	120.64
1	B	148	ALA	CA-C-O	-5.22	116.10	122.41
1	B	243	CYS	O-C-N	5.21	128.92	123.03
1	D	366	TRP	CA-CB-CG	5.21	123.51	113.60
1	A	40	TRP	CA-C-N	5.21	130.35	123.00
1	A	40	TRP	C-N-CA	5.21	130.35	123.00
1	D	277	GLY	CA-C-N	-5.21	113.63	123.27
1	D	277	GLY	C-N-CA	-5.21	113.63	123.27
1	D	276	LYS	CA-C-O	5.21	126.62	120.58
1	A	106	SER	O-C-N	5.20	129.51	122.96
1	D	49	CYS	N-CA-C	-5.19	107.11	113.50
1	A	228	HIS	CA-C-N	-5.18	113.68	123.27
1	A	228	HIS	C-N-CA	-5.18	113.68	123.27
1	D	214	ASP	CA-CB-CG	-5.17	107.42	112.60
1	D	34	ILE	CA-C-N	5.17	128.19	120.90
1	D	34	ILE	C-N-CA	5.17	128.19	120.90
1	D	225	PHE	CA-CB-CG	5.16	118.96	113.80
1	D	365	ILE	CA-C-O	-5.16	115.08	120.76
1	C	66	ALA	CA-C-N	-5.14	112.50	122.06
1	C	66	ALA	C-N-CA	-5.14	112.50	122.06
1	C	336	PHE	CA-CB-CG	-5.14	108.66	113.80
1	B	4	GLY	CA-C-N	-5.13	114.17	122.23
1	B	4	GLY	C-N-CA	-5.13	114.17	122.23
1	B	256	CYS	O-C-N	5.13	129.72	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	THR	CA-C-N	5.12	129.18	120.88
1	A	397	THR	C-N-CA	5.12	129.18	120.88
1	C	342	PHE	CA-C-N	5.12	127.55	120.29
1	C	342	PHE	C-N-CA	5.12	127.55	120.29
1	C	283	SER	CA-C-N	-5.11	114.18	122.36
1	C	283	SER	C-N-CA	-5.11	114.18	122.36
1	B	342	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	234	GLU	CA-C-O	-5.11	115.44	121.16
1	D	302	ILE	O-C-N	-5.08	117.77	123.26
1	A	339	ARG	CD-NE-CZ	5.07	131.50	124.40
1	C	198	ASP	O-C-N	5.07	127.57	121.29
1	D	212	GLU	CA-C-N	-5.06	116.22	123.11
1	D	212	GLU	C-N-CA	-5.06	116.22	123.11
1	C	333	PHE	CA-CB-CG	-5.05	108.75	113.80
1	D	147	VAL	CA-C-N	-5.03	114.53	122.08
1	D	147	VAL	C-N-CA	-5.03	114.53	122.08
1	D	342	PHE	CA-C-O	5.02	126.09	120.82
1	C	358	PRO	CA-C-O	-5.00	115.63	121.34
1	C	385	GLU	O-C-N	-5.00	116.68	123.19
1	C	52	GLY	CA-C-N	-5.00	115.21	122.86
1	C	52	GLY	C-N-CA	-5.00	115.21	122.86

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	3333	0	3028	277	0
1	B	3333	0	3028	319	0
1	C	3333	0	3028	146	0
1	D	3333	0	3030	113	0
2	A	139	0	0	15	0
2	B	147	0	0	18	0
2	C	187	0	0	14	0
2	D	216	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14021	0	12114	827	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 33.

All (827) 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:21:ALA:HB3	1:A:24:ASN:HD22	1.25	1.00
1:A:90:LEU:HD23	1:A:363:MET:HE3	1.52	0.91
1:A:141:ASN:HD21	1:A:217:GLU:HG2	1.33	0.90
1:B:2:ARG:HB2	1:B:70:MET:HG2	1.54	0.89
1:C:22:PRO:HD3	1:C:426:SER:HA	1.56	0.86
1:B:287:THR:HB	1:B:302:ILE:HB	1.58	0.86
1:A:95:VAL:HG22	1:A:104:VAL:HG22	1.56	0.85
1:B:318:MET:HE2	1:B:335:VAL:HG21	1.58	0.85
1:B:115:ASP:HA	1:B:166:ARG:HG3	1.59	0.84
1:A:132:ASP:HB2	1:A:285:LYS:HD3	1.60	0.84
1:D:59:CYS:HG	1:D:65:CYS:HG	0.97	0.83
1:B:99:GLU:HG3	1:C:40:TRP:HB2	1.61	0.82
1:C:379:ILE:HG21	1:C:385:GLU:HG3	1.61	0.82
1:A:295:ASN:H	1:A:352:ASN:HD21	1.27	0.82
1:A:128:ALA:HB2	1:A:289:VAL:HG13	1.61	0.81
1:B:163:ALA:HB1	1:B:167:TYR:HB2	1.61	0.80
1:B:155:MET:HE2	1:B:164:GLY:HA3	1.62	0.80
1:C:295:ASN:H	1:C:352:ASN:HD21	1.27	0.79
1:A:381:PRO:HB2	1:A:383:GLU:HG3	1.65	0.79
1:B:218:SER:HB3	1:B:223:PHE:HA	1.65	0.79
1:A:34:ILE:HG22	1:A:39:ARG:HH21	1.46	0.78
1:A:3:ALA:HB1	1:A:167:TYR:OH	1.83	0.78
1:B:144:LEU:HD12	1:B:363:MET:HG2	1.66	0.77
1:D:227:PRO:HD2	1:D:261:CYS:O	1.84	0.77
1:C:195:SER:HB3	1:C:198:ASP:O	1.86	0.76
1:D:125:ASN:HD22	1:D:423:PRO:HA	1.50	0.76
1:A:227:PRO:HD2	1:A:261:CYS:O	1.84	0.76
1:B:252:PHE:HA	2:B:434:HOH:O	1.84	0.75
1:B:173:ASP:HB2	1:B:212:GLU:OE1	1.86	0.75
1:B:267:ARG:HG3	1:B:392:ARG:HG2	1.67	0.74
1:B:408:GLN:O	1:B:410:PRO:HD3	1.87	0.74
1:B:265:PRO:HA	1:B:268:MET:HB2	1.70	0.73
1:D:64:ASP:O	1:D:68:LYS:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:TRP:HB3	1:B:189:ILE:HD12	1.69	0.73
1:C:419:ILE:HD12	1:C:419:ILE:H	1.54	0.73
1:A:105:GLY:HA2	1:A:365:ILE:HG23	1.72	0.72
1:A:198:ASP:OD2	1:A:201:ALA:HB3	1.89	0.72
1:B:364:SER:HB2	2:B:566:HOH:O	1.88	0.72
1:D:327:GLU:O	1:D:331:THR:HG23	1.88	0.72
1:A:122:LEU:O	1:A:125:ASN:HB2	1.89	0.72
1:A:218:SER:HA	1:A:376:LEU:HD21	1.72	0.72
1:A:374:LEU:HD22	1:A:379:ILE:O	1.90	0.72
1:A:145:TYR:HB2	1:A:213:ILE:O	1.90	0.72
1:A:189:ILE:HG23	1:A:190:GLU:H	1.55	0.72
1:A:331:THR:O	1:A:335:VAL:HG23	1.89	0.72
1:B:8:PRO:HG2	1:C:78:LEU:HD11	1.72	0.72
1:C:297:LEU:HD11	1:C:355:LEU:HD11	1.71	0.71
1:B:267:ARG:HA	1:B:391:ALA:O	1.91	0.71
1:A:361:LEU:HD12	1:A:362:VAL:H	1.55	0.71
1:B:420:ARG:HB3	1:B:427:THR:HG22	1.70	0.71
1:A:116:LYS:HB2	1:A:151:GLU:HG2	1.71	0.71
1:B:214:ASP:HB2	1:B:226:THR:O	1.91	0.70
1:A:340:ASN:O	1:A:344:GLU:HG3	1.92	0.70
1:C:169:THR:HG22	2:C:565:HOH:O	1.91	0.70
1:A:5:ASN:H	1:A:70:MET:HE3	1.57	0.70
1:B:150:GLU:HG3	2:B:466:HOH:O	1.91	0.70
1:B:5:ASN:ND2	1:B:70:MET:HE1	2.06	0.69
1:A:4:GLY:HA2	1:A:70:MET:SD	2.33	0.69
1:B:2:ARG:HA	1:B:162:GLN:HB2	1.75	0.69
1:A:178:ARG:HG3	1:A:247:TYR:HB2	1.74	0.69
1:C:328:LEU:O	1:C:332:MET:HG3	1.93	0.69
1:A:132:ASP:HB3	1:A:415:VAL:HB	1.73	0.69
1:B:96:THR:O	1:B:102:THR:HA	1.91	0.69
1:B:111:MET:HB3	1:B:116:LYS:O	1.92	0.69
1:B:287:THR:HG23	2:B:521:HOH:O	1.92	0.69
1:C:155:MET:HE2	2:C:566:HOH:O	1.93	0.69
1:D:26:GLN:HB2	2:D:516:HOH:O	1.93	0.69
1:A:262:ASP:OD1	1:A:332:MET:HE1	1.91	0.69
1:B:76:ASP:HB3	1:C:76:ASP:OD2	1.93	0.69
1:C:11:HIS:HB3	1:C:32:VAL:O	1.93	0.69
1:B:408:GLN:HG3	1:B:409:PHE:H	1.57	0.68
1:C:82:GLY:HA3	1:C:96:THR:HG21	1.73	0.68
1:B:5:ASN:HD21	1:B:70:MET:HE1	1.59	0.68
1:B:53:ASN:HB3	1:B:201:ALA:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HD21	1:B:361:LEU:HD11	1.75	0.68
1:A:291:ARG:O	1:A:297:LEU:HA	1.93	0.68
1:B:91:THR:OG1	1:B:415:VAL:HG22	1.94	0.68
1:D:85:THR:HG23	2:D:619:HOH:O	1.92	0.68
1:C:144:LEU:HD21	1:C:361:LEU:HD11	1.74	0.68
1:A:257:ASP:HA	1:A:341:ARG:HG2	1.74	0.68
1:B:47:GLN:OE1	1:B:58:ALA:HB2	1.93	0.68
1:D:18:ARG:HH11	1:D:18:ARG:HB2	1.59	0.68
1:A:34:ILE:HG22	1:A:39:ARG:NH2	2.08	0.67
1:B:147:VAL:HG21	1:B:171:TYR:HE1	1.60	0.67
1:D:340:ASN:ND2	1:D:343:GLU:H	1.91	0.67
1:A:48:ASN:HB3	1:A:50:TYR:O	1.93	0.67
1:B:175:GLN:HG3	1:B:258:ALA:HB1	1.76	0.67
1:A:287:THR:HB	1:A:302:ILE:HB	1.77	0.67
1:C:384:LYS:HG2	1:C:387:GLN:HE22	1.60	0.67
1:A:173:ASP:HB2	1:A:212:GLU:OE1	1.95	0.67
1:D:4:GLY:HA3	1:D:72:GLU:OE2	1.94	0.66
1:B:124:GLY:O	1:B:424:ILE:HD12	1.95	0.66
1:A:21:ALA:HB3	1:A:24:ASN:ND2	2.05	0.66
1:B:331:THR:O	1:B:334:ASP:HB2	1.95	0.66
1:B:76:ASP:HB3	1:C:76:ASP:HA	1.78	0.66
1:B:328:LEU:HD22	1:B:332:MET:HG3	1.76	0.66
1:C:74:ALA:HB1	1:C:81:TYR:HE2	1.60	0.66
1:C:115:ASP:HB2	2:C:585:HOH:O	1.96	0.66
1:D:95:VAL:HG22	1:D:104:VAL:HG22	1.78	0.65
1:A:341:ARG:HA	1:A:344:GLU:HG3	1.79	0.65
1:B:245:GLY:HA2	1:B:258:ALA:HB2	1.79	0.65
1:D:123:MET:HB3	2:D:535:HOH:O	1.95	0.65
1:A:149:MET:HE3	1:A:171:TYR:HA	1.79	0.65
1:B:426:SER:HB3	2:B:478:HOH:O	1.95	0.65
1:A:141:ASN:ND2	1:A:217:GLU:HG2	2.09	0.65
1:A:92:LEU:HD22	1:A:106:SER:OG	1.97	0.64
1:B:90:LEU:HD23	1:B:363:MET:SD	2.37	0.64
1:A:188:ASN:OD1	1:A:205:PRO:HD2	1.96	0.64
1:B:190:GLU:O	1:B:205:PRO:HD3	1.98	0.64
1:C:93:LYS:NZ	1:C:96:THR:HB	2.13	0.64
1:C:64:ASP:O	1:C:68:LYS:HG3	1.97	0.64
1:B:368:ASP:OD1	1:B:370:TYR:HB2	1.98	0.63
1:B:39:ARG:HD3	1:B:72:GLU:O	1.99	0.63
1:B:288:VAL:HG12	2:B:431:HOH:O	1.97	0.63
1:D:98:HIS:HE1	1:D:103:ASN:HB2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HB3	2:A:511:HOH:O	1.97	0.63
1:C:239:GLU:HG3	1:C:240:THR:HG23	1.80	0.63
1:B:195:SER:HA	2:B:573:HOH:O	1.98	0.63
1:A:52:GLY:O	1:A:200:ASN:HA	1.99	0.63
1:B:97:LYS:HA	1:B:102:THR:HA	1.79	0.63
1:B:147:VAL:HG22	1:B:362:VAL:HG21	1.80	0.63
1:D:41:LEU:HD12	1:D:181:LYS:NZ	2.14	0.63
1:A:423:PRO:HB3	2:A:524:HOH:O	1.99	0.62
1:A:195:SER:HA	2:A:520:HOH:O	1.98	0.62
1:D:41:LEU:HD12	1:D:181:LYS:HZ1	1.64	0.62
1:B:4:GLY:CA	1:B:70:MET:HE2	2.29	0.62
1:A:333:PHE:O	1:A:337:ASN:HA	1.99	0.62
1:C:384:LYS:HE2	2:C:477:HOH:O	2.00	0.62
1:B:29:ASN:H	1:B:29:ASN:ND2	1.95	0.62
1:A:219:ASN:HD21	1:A:221:TYR:HB2	1.64	0.62
1:C:41:LEU:HG	1:C:71:ILE:HG12	1.81	0.62
1:D:189:ILE:HG23	1:D:190:GLU:HG3	1.81	0.62
1:C:309:GLU:HG2	2:C:467:HOH:O	1.99	0.62
1:A:80:THR:HG23	1:A:98:HIS:CE1	2.35	0.62
1:B:143:ALA:HB3	1:B:364:SER:OG	1.99	0.62
1:B:209:CYS:HB2	1:B:236:HIS:CE1	2.35	0.62
1:C:383:GLU:O	1:C:384:LYS:HB2	2.00	0.62
1:D:331:THR:HA	1:D:334:ASP:OD1	2.00	0.62
1:A:361:LEU:HD12	1:A:362:VAL:N	2.15	0.62
1:A:208:SER:HB2	1:A:235:TYR:CE1	2.35	0.61
1:A:41:LEU:HG	1:A:71:ILE:HG22	1.82	0.61
1:A:178:ARG:HG3	1:A:247:TYR:HD2	1.64	0.61
1:D:80:THR:HG23	1:D:98:HIS:CD2	2.35	0.61
1:A:250:ASP:OD2	1:A:253:ALA:HB2	2.01	0.61
1:D:178:ARG:HG2	1:D:206:TYR:O	2.00	0.61
1:A:1:PCA:OE	1:A:161:ASN:HB2	2.00	0.61
1:B:99:GLU:HA	1:C:40:TRP:CE3	2.36	0.61
1:B:349:GLU:O	1:B:352:ASN:HB2	2.01	0.61
1:B:212:GLU:O	1:B:228:HIS:HB2	2.01	0.60
1:A:274:TYR:CD1	1:A:280:LEU:HD12	2.36	0.60
1:B:121:ASN:HB2	2:B:548:HOH:O	2.01	0.60
1:B:405:VAL:HA	1:B:408:GLN:HG2	1.83	0.60
1:C:48:ASN:O	1:C:56:THR:HG21	2.00	0.60
1:B:119:MET:HE1	1:B:149:MET:O	2.01	0.60
1:B:122:LEU:HD22	1:B:359:MET:HG3	1.81	0.60
1:B:18:ARG:HD3	2:B:550:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLY:O	1:A:331:THR:HB	2.01	0.60
1:D:385:GLU:O	1:D:385:GLU:HG2	2.02	0.60
1:A:324:ILE:HG22	1:A:348:PHE:CE1	2.36	0.60
1:A:178:ARG:NH1	1:A:243:CYS:HB2	2.17	0.59
1:B:117:TYR:OH	1:B:168:GLY:HA2	2.03	0.59
1:C:82:GLY:CA	1:C:96:THR:HG21	2.32	0.59
1:A:288:VAL:HG13	1:A:301:PHE:CD2	2.37	0.59
1:B:55:TRP:CH2	1:B:187:ALA:HB1	2.37	0.59
1:C:12:PRO:HB3	1:C:85:THR:HG22	1.84	0.59
1:B:180:LEU:HD12	1:B:208:SER:OG	2.02	0.59
1:D:13:PRO:O	1:D:85:THR:HG21	2.02	0.59
1:B:183:VAL:HG11	1:B:206:TYR:HB3	1.84	0.59
1:C:124:GLY:O	1:C:424:ILE:HG12	2.02	0.59
1:B:264:ASN:O	1:B:268:MET:HG2	2.01	0.59
1:A:384:LYS:CB	1:A:387:GLN:HE21	2.16	0.59
1:B:295:ASN:H	1:B:352:ASN:HD21	1.51	0.59
1:D:41:LEU:HD11	1:D:182:PHE:HE2	1.68	0.58
1:A:315:TRP:HB2	1:A:318:MET:HG3	1.84	0.58
1:B:78:LEU:HD13	1:C:10:ASN:ND2	2.18	0.58
1:B:97:LYS:HE3	1:C:6:GLU:HA	1.83	0.58
1:C:125:ASN:HD22	1:C:423:PRO:HA	1.68	0.58
1:B:136:VAL:HG11	1:B:142:SER:OG	2.03	0.58
1:C:27:THR:HG22	1:C:29:ASN:HD21	1.67	0.58
1:D:213:ILE:HD11	1:D:359:MET:HE3	1.85	0.58
1:A:174:ALA:H	1:A:212:GLU:HB2	1.67	0.58
1:A:239:GLU:HA	1:A:239:GLU:OE1	2.03	0.58
1:B:8:PRO:HG2	1:C:78:LEU:CD1	2.34	0.58
1:A:127:LEU:HG	1:A:128:ALA:N	2.17	0.58
1:B:80:THR:HB	1:B:81:TYR:CD2	2.38	0.58
1:C:266:TYR:CD2	1:C:271:PRO:HA	2.38	0.58
1:B:97:LYS:HD2	1:C:6:GLU:OE1	2.03	0.58
1:D:125:ASN:HD22	1:D:423:PRO:CA	2.16	0.58
1:A:356:ARG:HB3	1:B:24:ASN:HD21	1.69	0.58
1:B:55:TRP:CB	1:B:189:ILE:HD12	2.34	0.58
1:D:54:GLN:HG3	1:D:194:SER:OG	2.04	0.58
1:B:6:GLU:HB2	1:B:72:GLU:OE2	2.04	0.57
1:B:230:CYS:HB2	1:B:232:THR:O	2.04	0.57
1:B:78:LEU:HG	1:B:84:SER:HB3	1.84	0.57
1:B:126:GLU:OE1	1:B:291:ARG:HG2	2.04	0.57
1:C:59:CYS:HA	1:C:68:LYS:HZ3	1.68	0.57
1:C:78:LEU:HG	1:C:84:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASP:HB2	1:B:56:THR:CG2	2.34	0.57
1:B:205:PRO:O	1:B:206:TYR:HD2	1.87	0.57
1:B:141:ASN:HD21	1:B:217:GLU:HB3	1.69	0.57
1:B:377:ASP:HB2	1:B:395:CYS:SG	2.45	0.57
1:C:59:CYS:HA	1:C:68:LYS:NZ	2.20	0.57
1:C:385:GLU:HG2	1:C:386:GLY:N	2.18	0.57
1:B:146:PHE:HB3	1:B:359:MET:HB3	1.85	0.57
1:B:245:GLY:HA2	1:B:258:ALA:CB	2.34	0.57
1:C:13:PRO:O	1:C:85:THR:HG21	2.04	0.57
1:D:148:ALA:HB3	1:D:210:CYS:HB2	1.87	0.57
1:B:373:MET:SD	1:B:376:LEU:HD23	2.45	0.57
1:D:50:TYR:OH	1:D:53:ASN:HA	2.04	0.57
1:A:209:CYS:O	1:A:235:TYR:HA	2.05	0.57
1:A:324:ILE:HG22	1:A:348:PHE:CZ	2.40	0.57
1:B:226:THR:HG1	1:B:262:ASP:HA	1.69	0.57
1:B:209:CYS:O	1:B:210:CYS:HB3	2.05	0.57
1:A:172:CYS:SG	1:A:235:TYR:HD1	2.28	0.56
1:C:19:CYS:HA	1:C:25:CYS:HA	1.87	0.56
1:D:18:ARG:HH11	1:D:18:ARG:CB	2.18	0.56
1:D:85:THR:HA	2:D:578:HOH:O	2.05	0.56
1:B:295:ASN:HA	1:B:348:PHE:CE2	2.41	0.56
1:C:63:THR:OG1	1:C:186:LYS:HE2	2.05	0.56
1:D:188:ASN:OD1	1:D:205:PRO:HD2	2.04	0.56
1:A:127:LEU:HD23	2:A:534:HOH:O	2.05	0.56
1:A:267:ARG:HA	1:A:391:ALA:O	2.04	0.56
1:A:368:ASP:HB2	1:A:373:MET:CE	2.35	0.56
1:B:68:LYS:HZ2	1:B:68:LYS:HB3	1.70	0.56
1:A:144:LEU:HG	1:A:363:MET:HG3	1.87	0.56
1:A:178:ARG:HG3	1:A:247:TYR:CD2	2.40	0.56
1:B:333:PHE:HE2	1:B:338:ASP:HB2	1.70	0.56
1:A:90:LEU:HD12	1:A:91:THR:N	2.21	0.56
1:A:158:TYR:HB3	1:A:184:GLY:O	2.06	0.56
1:C:380:TYR:CD1	1:C:381:PRO:HA	2.40	0.56
1:D:16:TRP:HH2	2:D:579:HOH:O	1.88	0.56
1:B:244:GLY:HA2	1:B:248:SER:HB2	1.87	0.56
1:A:155:MET:HG2	1:A:161:ASN:O	2.06	0.56
1:A:38:TRP:CZ2	1:A:106:SER:HA	2.41	0.56
1:A:252:PHE:CD1	1:A:339:ARG:HD3	2.40	0.56
1:B:219:ASN:OD1	1:B:376:LEU:HD21	2.06	0.55
1:A:270:ASN:HB3	2:A:488:HOH:O	2.06	0.55
1:B:218:SER:HB3	1:B:223:PHE:CA	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:TYR:CD1	1:B:268:MET:HE3	2.41	0.55
1:C:27:THR:HG22	1:C:29:ASN:ND2	2.21	0.55
1:C:74:ALA:HB1	1:C:81:TYR:CE2	2.41	0.55
1:A:21:ALA:HB1	1:A:22:PRO:HD2	1.87	0.55
1:B:333:PHE:CE2	1:B:338:ASP:HB2	2.42	0.55
1:D:241:THR:HG22	1:D:249:GLU:OE1	2.06	0.55
1:A:266:TYR:HB2	2:A:541:HOH:O	2.05	0.55
1:B:144:LEU:HA	1:B:362:VAL:O	2.06	0.55
1:B:266:TYR:CD2	1:B:271:PRO:HA	2.41	0.55
1:D:295:ASN:H	1:D:352:ASN:HD21	1.53	0.55
1:A:132:ASP:HB3	1:A:415:VAL:CB	2.36	0.55
1:B:198:ASP:OD1	1:B:199:PRO:HD2	2.06	0.55
1:B:188:ASN:O	1:B:192:TRP:HE3	1.90	0.55
1:C:400:GLY:HA2	1:C:405:VAL:HG11	1.88	0.55
1:D:307:LYS:HE3	1:D:430:PHE:HB3	1.89	0.55
1:C:404:GLU:O	1:C:408:GLN:HG2	2.06	0.55
1:A:144:LEU:CD2	1:A:361:LEU:HD11	2.37	0.55
1:B:263:TYR:CE1	1:B:268:MET:HG3	2.42	0.55
1:C:7:THR:HG22	1:C:8:PRO:O	2.06	0.55
1:B:55:TRP:CD2	1:B:189:ILE:HB	2.42	0.55
1:B:231:THR:OG1	1:B:255:LYS:HB3	2.07	0.54
1:B:379:ILE:HG21	1:B:385:GLU:HB2	1.89	0.54
1:B:97:LYS:HA	1:B:102:THR:OG1	2.07	0.54
1:D:34:ILE:HB	1:D:77:TYR:HE2	1.71	0.54
1:D:379:ILE:HG21	1:D:385:GLU:HB2	1.89	0.54
1:A:139:GLY:CA	1:A:400:GLY:HA2	2.37	0.54
1:A:139:GLY:HA3	1:A:400:GLY:HA2	1.90	0.54
1:A:147:VAL:HG12	1:A:212:GLU:HG3	1.88	0.54
1:A:315:TRP:HB2	1:A:318:MET:SD	2.47	0.54
1:D:40:TRP:CE3	1:D:72:GLU:HG3	2.42	0.54
1:B:12:PRO:HD3	1:B:77:TYR:CE1	2.43	0.54
1:B:64:ASP:O	1:B:67:GLU:HB2	2.07	0.54
1:D:96:THR:OG1	1:D:103:ASN:HB3	2.08	0.54
1:B:149:MET:HB2	1:B:360:VAL:HG21	1.90	0.54
1:C:93:LYS:HE3	1:C:96:THR:CG2	2.37	0.54
1:D:35:ASP:HB3	1:D:38:TRP:CE3	2.43	0.54
1:A:368:ASP:HB2	1:A:373:MET:HE2	1.89	0.54
1:B:76:ASP:H	1:C:76:ASP:CG	2.15	0.54
1:B:152:ASP:OD2	1:B:155:MET:HB2	2.08	0.54
1:A:42:HIS:CE1	1:A:70:MET:HE2	2.43	0.54
1:B:147:VAL:CG1	1:B:212:GLU:HG3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:GLU:HA	1:B:316:GLU:OE1	2.06	0.54
1:D:50:TYR:CD1	1:D:181:LYS:HD2	2.42	0.54
1:A:6:GLU:O	1:D:97:LYS:HG3	2.08	0.54
1:A:6:GLU:OE2	1:A:42:HIS:HE1	1.91	0.54
1:A:380:TYR:HB3	1:A:392:ARG:NE	2.23	0.54
1:B:81:TYR:O	1:B:96:THR:HG21	2.08	0.54
1:B:209:CYS:HB2	1:B:236:HIS:NE2	2.23	0.54
1:D:379:ILE:HD13	1:D:385:GLU:HG3	1.90	0.54
1:A:137:GLU:HG3	1:A:409:PHE:CE1	2.43	0.53
1:B:287:THR:O	1:B:301:PHE:HA	2.07	0.53
1:D:293:GLU:HG3	1:D:424:ILE:HD11	1.90	0.53
1:C:384:LYS:HG2	1:C:387:GLN:NE2	2.22	0.53
1:A:68:LYS:NZ	1:A:68:LYS:HB3	2.16	0.53
1:A:292:PHE:HB3	1:A:355:LEU:HD22	1.90	0.53
1:B:23:GLY:O	1:B:24:ASN:HB2	2.09	0.53
1:B:267:ARG:HD3	1:B:336:PHE:CE2	2.43	0.53
1:A:64:ASP:O	1:A:68:LYS:HG2	2.08	0.53
1:A:263:TYR:CZ	1:A:322:SER:HA	2.43	0.53
1:B:36:ALA:O	1:B:39:ARG:HB2	2.09	0.53
1:A:112:ASN:HB2	1:A:118:GLN:HB2	1.90	0.53
1:A:172:CYS:HA	1:A:208:SER:OG	2.09	0.53
1:D:48:ASN:O	1:D:56:THR:HG21	2.08	0.53
1:A:401:VAL:HG23	2:A:548:HOH:O	2.09	0.53
1:C:327:GLU:O	1:C:331:THR:HG23	2.09	0.53
1:D:80:THR:HG23	1:D:98:HIS:NE2	2.24	0.53
1:A:15:THR:HB	1:A:27:THR:CG2	2.38	0.53
1:A:178:ARG:HH22	1:A:240:THR:HA	1.74	0.53
1:A:372:ASN:O	1:A:400:GLY:HA3	2.09	0.53
1:B:147:VAL:HG21	1:B:171:TYR:CE1	2.40	0.53
1:A:92:LEU:O	1:A:413:GLN:HB2	2.09	0.53
1:A:295:ASN:H	1:A:352:ASN:ND2	2.03	0.53
1:A:332:MET:HE3	1:A:336:PHE:CE2	2.44	0.53
1:A:363:MET:HG2	1:A:416:TRP:CD1	2.44	0.53
1:B:275:GLY:C	1:B:278:LYS:HG3	2.33	0.53
1:A:271:PRO:HD2	1:A:272:ASP:OD1	2.09	0.52
1:C:9:GLU:OE2	1:C:9:GLU:HA	2.08	0.52
1:D:249:GLU:HG3	2:D:580:HOH:O	2.09	0.52
1:B:185:GLY:C	1:B:186:LYS:HE3	2.34	0.52
1:A:137:GLU:HG3	1:A:409:PHE:CD1	2.44	0.52
1:A:210:CYS:HB3	1:A:235:TYR:HA	1.92	0.52
1:B:134:SER:HB3	1:B:283:SER:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASP:CG	1:B:260:GLY:H	2.18	0.52
1:C:148:ALA:HB3	1:C:210:CYS:HB2	1.92	0.52
1:D:82:GLY:O	1:D:93:LYS:HD3	2.08	0.52
1:A:315:TRP:HB2	1:A:318:MET:CG	2.40	0.52
1:A:76:ASP:OD2	1:D:76:ASP:HB3	2.09	0.52
1:B:96:THR:HG23	1:B:103:ASN:HB3	1.91	0.52
1:A:155:MET:HE1	1:A:166:ARG:NE	2.25	0.52
1:B:302:ILE:O	1:B:302:ILE:HG22	2.09	0.52
1:C:269:GLY:HA3	1:C:314:THR:OG1	2.09	0.52
1:D:71:ILE:HD12	1:D:167:TYR:HB3	1.91	0.52
1:A:341:ARG:O	1:A:344:GLU:HB2	2.10	0.52
1:B:51:ASP:HB2	1:B:56:THR:HG22	1.92	0.52
1:B:341:ARG:HA	1:B:344:GLU:OE2	2.10	0.52
1:A:176:CYS:HA	1:A:208:SER:O	2.10	0.52
1:B:3:ALA:O	1:B:4:GLY:O	2.28	0.52
1:A:109:TYR:CD1	1:A:362:VAL:HG13	2.44	0.51
1:A:128:ALA:HB1	1:A:428:TYR:HE1	1.75	0.51
1:A:172:CYS:O	1:A:173:ASP:HB3	2.10	0.51
1:B:98:HIS:CD2	1:B:100:TYR:H	2.27	0.51
1:A:60:SER:O	1:A:189:ILE:HD13	2.09	0.51
1:A:149:MET:HE3	1:A:171:TYR:CA	2.39	0.51
1:A:266:TYR:CD2	1:A:393:GLY:HA2	2.46	0.51
1:B:367:ASP:HB2	2:B:531:HOH:O	2.09	0.51
1:C:114:PRO:O	1:C:166:ARG:HG2	2.10	0.51
1:C:55:TRP:CZ2	1:C:181:LYS:HB3	2.45	0.51
1:D:311:PRO:HG3	2:D:551:HOH:O	2.10	0.51
1:B:350:GLN:O	1:B:353:ASN:HB2	2.10	0.51
1:C:328:LEU:HD22	1:C:332:MET:HG3	1.93	0.51
1:D:241:THR:HG22	1:D:249:GLU:CD	2.36	0.51
1:A:45:ASN:O	1:A:46:MET:HB2	2.10	0.51
1:B:163:ALA:O	1:B:166:ARG:HD3	2.11	0.51
1:A:365:ILE:O	1:A:366:TRP:HB3	2.11	0.51
1:B:163:ALA:HB1	1:B:167:TYR:CB	2.38	0.51
1:B:290:SER:OG	1:B:299:GLN:HG3	2.11	0.51
1:B:327:GLU:O	1:B:330:SER:OG	2.29	0.51
1:C:41:LEU:HD12	2:C:466:HOH:O	2.11	0.51
1:A:92:LEU:HD21	1:A:108:PHE:CD1	2.46	0.51
1:A:268:MET:HA	1:A:315:TRP:HE1	1.76	0.51
1:A:356:ARG:HB3	1:B:24:ASN:ND2	2.26	0.51
1:B:263:TYR:HD1	1:B:268:MET:HE3	1.76	0.51
1:C:275:GLY:O	1:C:281:ASP:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:GLY:N	1:B:70:MET:HE2	2.26	0.51
1:A:78:LEU:HD21	1:D:8:PRO:HD2	1.93	0.50
1:A:15:THR:OG1	1:A:88:ASP:HB3	2.11	0.50
1:A:160:SER:OG	1:A:185:GLY:O	2.29	0.50
1:A:341:ARG:HD2	1:A:344:GLU:OE1	2.11	0.50
1:C:217:GLU:O	1:C:223:PHE:HA	2.12	0.50
1:A:3:ALA:HB1	1:A:167:TYR:CZ	2.45	0.50
1:B:95:VAL:HG23	1:B:410:PRO:HA	1.94	0.50
1:D:53:ASN:CG	1:D:194:SER:HB3	2.36	0.50
1:C:268:MET:O	1:C:313:PRO:HA	2.11	0.50
1:A:102:THR:O	1:A:102:THR:HG22	2.12	0.50
1:B:53:ASN:OD1	1:B:199:PRO:O	2.30	0.50
1:B:65:CYS:SG	1:B:189:ILE:HG21	2.50	0.50
1:B:365:ILE:HG23	1:B:365:ILE:O	2.11	0.50
1:A:125:ASN:HD21	1:B:18:ARG:HH12	1.58	0.50
1:A:178:ARG:O	1:A:203:VAL:HA	2.12	0.50
1:A:219:ASN:CG	1:A:221:TYR:H	2.20	0.50
1:B:61:THR:O	1:B:64:ASP:OD2	2.30	0.50
1:C:383:GLU:HA	1:C:383:GLU:OE2	2.12	0.50
1:C:429:ASP:C	1:D:284:ARG:HH22	2.19	0.50
1:D:41:LEU:HD22	1:D:69:CYS:HB3	1.94	0.50
1:A:76:ASP:CG	1:D:76:ASP:H	2.20	0.50
1:A:128:ALA:CB	1:A:289:VAL:HG13	2.37	0.50
1:B:346:GLY:HA3	1:B:350:GLN:HB2	1.94	0.50
1:A:35:ASP:OD1	1:A:109:TYR:OH	2.30	0.50
1:A:377:ASP:O	1:A:393:GLY:HA3	2.12	0.50
1:A:379:ILE:O	1:A:379:ILE:HG22	2.12	0.50
1:A:384:LYS:O	1:A:385:GLU:O	2.30	0.50
1:B:76:ASP:OD1	1:C:75:GLY:O	2.30	0.50
1:B:295:ASN:O	1:B:296:LYS:HB2	2.12	0.50
1:D:90:LEU:HD21	1:D:92:LEU:HD21	1.93	0.50
1:D:241:THR:HG22	1:D:249:GLU:OE2	2.12	0.50
1:C:143:ALA:HB3	1:C:364:SER:OG	2.12	0.49
1:D:333:PHE:O	1:D:336:PHE:O	2.30	0.49
1:A:29:ASN:HB3	2:A:553:HOH:O	2.12	0.49
1:A:132:ASP:CB	1:A:285:LYS:HD3	2.35	0.49
1:A:141:ASN:HD21	1:A:217:GLU:CG	2.16	0.49
1:A:295:ASN:OD1	1:A:352:ASN:OD1	2.29	0.49
1:B:95:VAL:HG12	1:B:102:THR:HG23	1.95	0.49
1:B:244:GLY:HA2	1:B:250:ASP:O	2.12	0.49
1:C:306:ARG:HH12	1:D:418:ASN:ND2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:CYS:HA	1:A:24:ASN:O	2.13	0.49
1:A:47:GLN:HG2	1:A:58:ALA:HB2	1.93	0.49
1:A:144:LEU:HD21	1:A:361:LEU:HD11	1.94	0.49
1:C:40:TRP:HB3	1:C:72:GLU:HB2	1.92	0.49
1:D:318:MET:HE1	1:D:336:PHE:CZ	2.48	0.49
1:A:53:ASN:HB3	1:A:201:ALA:N	2.28	0.49
1:A:121:ASN:O	1:A:125:ASN:OD1	2.30	0.49
1:B:299:GLN:O	1:B:310:ILE:HD11	2.11	0.49
1:B:32:VAL:HG12	1:B:110:LEU:HA	1.95	0.49
1:B:96:THR:OG1	1:B:103:ASN:HB3	2.13	0.49
1:B:152:ASP:CG	1:B:155:MET:HB2	2.37	0.49
1:B:303:GLN:O	1:B:304:ASP:HB2	2.12	0.49
1:B:361:LEU:HD12	1:B:362:VAL:N	2.27	0.49
1:B:198:ASP:HB3	1:B:201:ALA:HB3	1.94	0.49
1:B:323:GLU:HA	2:B:448:HOH:O	2.12	0.49
1:A:39:ARG:HD3	1:A:72:GLU:O	2.11	0.49
1:C:6:GLU:HB2	1:C:72:GLU:OE2	2.12	0.49
1:A:315:TRP:CH2	1:A:388:PRO:HA	2.47	0.49
1:B:263:TYR:OH	1:B:311:PRO:O	2.30	0.49
1:C:63:THR:HG21	2:C:593:HOH:O	2.12	0.49
1:A:356:ARG:HA	2:A:557:HOH:O	2.13	0.49
1:B:226:THR:HG23	1:B:262:ASP:N	2.28	0.49
1:C:15:THR:O	1:C:419:ILE:HD13	2.13	0.49
1:C:144:LEU:CD2	1:C:361:LEU:HD11	2.43	0.49
1:C:349:GLU:OE2	1:C:349:GLU:O	2.31	0.49
1:A:43:ASP:OD1	1:A:45:ASN:OD1	2.30	0.48
1:A:198:ASP:HB3	1:A:369:HIS:CD2	2.48	0.48
1:A:295:ASN:ND2	1:A:326:PRO:HG2	2.28	0.48
1:B:226:THR:OG1	1:B:262:ASP:HA	2.13	0.48
1:C:295:ASN:H	1:C:352:ASN:ND2	2.05	0.48
1:A:163:ALA:O	1:A:166:ARG:HG3	2.13	0.48
1:A:384:LYS:HG2	1:A:387:GLN:NE2	2.27	0.48
1:A:402:PRO:O	1:A:406:GLU:HG3	2.13	0.48
1:B:76:ASP:CG	1:C:76:ASP:HA	2.38	0.48
1:B:291:ARG:HB3	1:B:424:ILE:HG12	1.94	0.48
1:C:55:TRP:HB3	1:C:189:ILE:HD12	1.94	0.48
1:A:143:ALA:HA	1:A:216:TRP:O	2.13	0.48
1:B:37:ASN:OD1	1:B:180:LEU:HA	2.13	0.48
1:B:122:LEU:HG	1:B:292:PHE:CE1	2.47	0.48
1:B:182:PHE:HD2	2:B:442:HOH:O	1.95	0.48
1:C:188:ASN:OD1	1:C:205:PRO:HD2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:TYR:CE1	1:D:181:LYS:HD2	2.47	0.48
1:A:95:VAL:HG22	1:A:104:VAL:CG2	2.37	0.48
1:D:175:GLN:O	1:D:245:GLY:HA3	2.13	0.48
1:A:325:THR:OG1	1:A:327:GLU:OE1	2.30	0.48
1:A:375:TRP:HA	1:A:392:ARG:HD3	1.95	0.48
1:B:74:ALA:HB3	1:B:77:TYR:CE1	2.49	0.48
1:A:234:GLU:CD	1:A:234:GLU:H	2.22	0.48
1:A:307:LYS:HE3	1:A:430:PHE:HB3	1.96	0.48
1:B:122:LEU:HG	1:B:292:PHE:CD1	2.48	0.48
1:D:125:ASN:HA	1:D:423:PRO:HA	1.96	0.48
1:A:113:GLY:HA3	2:A:451:HOH:O	2.14	0.48
1:B:15:THR:OG1	1:B:87:GLY:O	2.30	0.48
1:B:127:LEU:HD22	1:B:146:PHE:CE1	2.49	0.48
1:B:361:LEU:HD12	1:B:362:VAL:H	1.78	0.48
1:A:90:LEU:HD12	1:A:91:THR:H	1.78	0.48
1:A:214:ASP:HB2	1:A:226:THR:HB	1.96	0.48
1:B:40:TRP:CE3	1:B:72:GLU:HG3	2.49	0.48
1:B:136:VAL:HG13	1:B:140:ILE:CG2	2.44	0.48
1:C:227:PRO:HG3	1:C:297:LEU:HD22	1.95	0.48
1:A:84:SER:HB2	1:A:91:THR:HB	1.95	0.48
1:A:131:VAL:O	1:A:285:LYS:HG3	2.14	0.48
1:A:177:ALA:HB3	1:A:208:SER:OG	2.14	0.48
1:B:210:CYS:HB3	1:B:235:TYR:HA	1.95	0.48
1:D:252:PHE:HD2	1:D:341:ARG:HD3	1.79	0.48
1:A:366:TRP:HB3	2:A:457:HOH:O	2.14	0.48
1:B:227:PRO:HG3	1:B:297:LEU:HD23	1.96	0.48
1:B:239:GLU:HG3	1:B:240:THR:HG23	1.95	0.48
1:B:384:LYS:HG2	1:B:387:GLN:NE2	2.28	0.48
1:C:9:GLU:CD	1:C:39:ARG:HH12	2.22	0.48
1:B:72:GLU:OE1	1:B:72:GLU:HA	2.14	0.47
1:B:296:LYS:HE3	1:B:298:SER:OG	2.14	0.47
1:D:158:TYR:CD2	1:D:184:GLY:HA2	2.49	0.47
1:A:17:GLN:HB2	1:A:26:GLN:O	2.13	0.47
1:A:218:SER:CA	1:A:376:LEU:HD21	2.44	0.47
1:B:2:ARG:HD2	1:B:70:MET:CG	2.44	0.47
1:C:93:LYS:HZ2	1:C:96:THR:HB	1.78	0.47
1:C:319:PRO:CG	1:C:328:LEU:HD23	2.44	0.47
1:D:59:CYS:HG	1:D:65:CYS:CB	2.24	0.47
1:A:20:THR:HB	1:B:112:ASN:OD1	2.14	0.47
1:A:297:LEU:CD1	1:A:355:LEU:HD11	2.45	0.47
1:D:348:PHE:CE2	1:D:351:LEU:HD23	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLY:HA2	1:A:281:ASP:CG	2.39	0.47
1:B:4:GLY:HA2	1:B:70:MET:HE2	1.97	0.47
1:B:269:GLY:O	1:B:271:PRO:HD3	2.15	0.47
1:B:380:TYR:HB3	1:B:392:ARG:NE	2.30	0.47
1:C:12:PRO:HB2	1:C:32:VAL:HG23	1.97	0.47
1:B:261:CYS:SG	1:B:332:MET:HE2	2.54	0.47
1:C:94:PHE:CD2	1:C:95:VAL:HG23	2.50	0.47
1:C:291:ARG:HB3	1:C:424:ILE:HD12	1.97	0.47
1:A:17:GLN:HA	1:A:28:VAL:HG23	1.97	0.47
1:A:155:MET:HG3	1:A:164:GLY:HA3	1.97	0.47
1:A:326:PRO:O	1:A:330:SER:OG	2.31	0.47
1:A:356:ARG:HG2	1:B:24:ASN:HD21	1.80	0.47
1:B:166:ARG:HH11	1:B:166:ARG:HB2	1.80	0.47
1:B:405:VAL:HA	1:B:408:GLN:CG	2.44	0.47
1:C:115:ASP:HA	1:C:166:ARG:HG2	1.96	0.47
1:B:65:CYS:O	1:B:69:CYS:HB2	2.15	0.47
1:B:155:MET:CE	1:B:164:GLY:HA3	2.41	0.47
1:C:53:ASN:O	1:C:194:SER:OG	2.30	0.47
1:D:155:MET:HE3	1:D:155:MET:HB3	1.75	0.47
1:A:396:PRO:O	1:A:399:SER:OG	2.30	0.47
1:B:64:ASP:HA	1:B:67:GLU:OE1	2.15	0.47
1:B:126:GLU:HB2	1:B:290:SER:O	2.14	0.47
1:A:37:ASN:OD1	1:A:181:LYS:HD2	2.15	0.47
1:A:372:ASN:HB3	1:A:400:GLY:HA3	1.95	0.47
1:B:13:PRO:O	1:B:85:THR:HG21	2.15	0.47
1:A:5:ASN:H	1:A:70:MET:CE	2.24	0.46
1:A:43:ASP:HB2	2:A:489:HOH:O	2.15	0.46
1:A:125:ASN:HB3	1:A:421:PHE:CZ	2.50	0.46
1:B:112:ASN:O	1:B:116:LYS:HE2	2.16	0.46
1:B:141:ASN:HB2	1:B:373:MET:HE3	1.96	0.46
1:B:360:VAL:O	1:B:362:VAL:HG23	2.15	0.46
1:D:49:CYS:C	1:D:56:THR:HG23	2.40	0.46
1:B:4:GLY:N	1:B:71:ILE:O	2.48	0.46
1:A:84:SER:CB	1:A:91:THR:HB	2.46	0.46
1:B:112:ASN:HB2	1:B:118:GLN:HA	1.95	0.46
1:B:177:ALA:HB3	1:B:180:LEU:HD12	1.97	0.46
1:B:297:LEU:HD22	1:B:348:PHE:HZ	1.80	0.46
1:C:6:GLU:HB2	1:C:72:GLU:CD	2.40	0.46
1:D:377:ASP:O	1:D:395:CYS:HB2	2.15	0.46
1:B:105:GLY:O	1:B:106:SER:HB3	2.16	0.46
1:C:61:THR:HG23	1:C:64:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:THR:OG1	1:C:64:ASP:OD2	2.30	0.46
1:C:367:ASP:OD2	1:C:406:GLU:OE2	2.32	0.46
1:D:367:ASP:OD2	1:D:406:GLU:OE2	2.34	0.46
1:A:378:SER:O	1:A:392:ARG:HB2	2.16	0.46
1:B:89:ALA:HA	1:B:416:TRP:O	2.15	0.46
1:C:18:ARG:HH11	1:C:18:ARG:HD2	1.54	0.46
1:D:147:VAL:HG23	1:D:149:MET:HG3	1.98	0.46
1:A:123:MET:HE2	1:A:355:LEU:CB	2.46	0.46
1:A:128:ALA:HB3	1:A:420:ARG:HG3	1.96	0.46
1:A:294:GLU:O	1:A:295:ASN:HB2	2.16	0.46
1:A:315:TRP:O	1:A:318:MET:HG3	2.16	0.46
1:B:384:LYS:O	1:B:385:GLU:O	2.33	0.46
1:D:380:TYR:CG	1:D:381:PRO:HA	2.50	0.46
1:A:92:LEU:HD21	1:A:108:PHE:CE1	2.51	0.46
1:B:2:ARG:HD2	1:B:70:MET:HG3	1.98	0.46
1:B:20:THR:O	1:B:21:ALA:HB2	2.15	0.46
1:C:285:LYS:NZ	2:C:509:HOH:O	2.48	0.46
1:D:291:ARG:HB3	1:D:424:ILE:HD13	1.97	0.46
1:A:74:ALA:HB1	1:A:81:TYR:CE2	2.51	0.45
1:A:223:PHE:CE2	1:A:265:PRO:HG2	2.50	0.45
1:B:37:ASN:OD1	1:B:180:LEU:HD23	2.16	0.45
1:C:405:VAL:HA	1:C:408:GLN:HG2	1.98	0.45
1:A:214:ASP:OD2	1:A:228:HIS:NE2	2.49	0.45
1:A:287:THR:HG21	1:A:428:TYR:CE1	2.51	0.45
1:B:218:SER:HB3	1:B:223:PHE:CB	2.46	0.45
1:B:291:ARG:NH2	1:B:430:PHE:OXT	2.49	0.45
1:B:357:VAL:HG13	1:B:358:PRO:HD2	1.98	0.45
1:A:20:THR:OG1	1:B:116:LYS:NZ	2.49	0.45
1:A:41:LEU:HA	1:A:70:MET:O	2.17	0.45
1:A:55:TRP:HE1	1:A:192:TRP:CG	2.34	0.45
1:B:78:LEU:O	1:B:82:GLY:N	2.50	0.45
1:B:324:ILE:O	1:B:324:ILE:HG22	2.15	0.45
1:A:124:GLY:O	1:A:125:ASN:ND2	2.50	0.45
1:B:66:ALA:HB2	1:B:182:PHE:HE1	1.81	0.45
1:B:80:THR:HB	1:B:81:TYR:CE2	2.52	0.45
1:B:116:LYS:HB3	1:B:151:GLU:HG2	1.98	0.45
1:B:121:ASN:N	2:B:548:HOH:O	2.50	0.45
1:B:328:LEU:HD22	1:B:332:MET:CG	2.44	0.45
1:C:270:ASN:ND2	2:C:600:HOH:O	2.50	0.45
1:D:329:CYS:O	1:D:333:PHE:HD1	2.00	0.45
1:A:133:LEU:O	1:A:220:ALA:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ILE:O	1:A:322:SER:OG	2.30	0.45
1:A:408:GLN:O	1:A:408:GLN:HG3	2.17	0.45
1:B:23:GLY:HA2	2:B:553:HOH:O	2.16	0.45
1:B:251:ARG:O	1:B:251:ARG:HG2	2.14	0.45
1:C:340:ASN:ND2	1:C:343:GLU:H	2.14	0.45
1:A:64:ASP:OD2	1:A:65:CYS:N	2.50	0.45
1:A:197:SER:OG	1:A:198:ASP:N	2.50	0.45
1:B:141:ASN:N	1:B:366:TRP:O	2.50	0.45
1:A:70:MET:HE3	1:A:72:GLU:OE2	2.16	0.45
1:A:217:GLU:O	1:A:218:SER:HB3	2.15	0.45
1:B:53:ASN:HD22	1:B:194:SER:HB3	1.80	0.45
1:D:307:LYS:HB2	1:D:430:PHE:CD2	2.52	0.45
1:A:2:ARG:HA	1:A:162:GLN:HG3	1.98	0.45
1:A:287:THR:HG21	1:A:428:TYR:CZ	2.52	0.45
1:A:357:VAL:O	1:A:359:MET:HG3	2.16	0.45
1:B:131:VAL:O	1:B:131:VAL:HG13	2.15	0.45
1:B:137:GLU:OE2	1:B:221:TYR:HE1	2.00	0.45
1:D:76:ASP:OD2	1:D:78:LEU:N	2.50	0.45
1:D:181:LYS:HE3	1:D:181:LYS:HB2	1.29	0.45
1:A:98:HIS:ND1	1:A:101:GLY:O	2.50	0.45
1:B:55:TRP:CD1	1:B:189:ILE:HA	2.52	0.45
1:B:98:HIS:N	1:B:101:GLY:O	2.50	0.45
1:B:139:GLY:HA3	1:B:400:GLY:HA2	1.98	0.45
1:B:154:GLY:O	1:B:158:TYR:HB2	2.16	0.45
1:B:275:GLY:O	1:B:278:LYS:HG3	2.17	0.45
1:D:93:LYS:HD2	2:D:589:HOH:O	2.16	0.45
1:D:98:HIS:O	1:D:100:TYR:N	2.50	0.45
1:B:64:ASP:O	1:B:67:GLU:N	2.50	0.45
1:D:2:ARG:NH1	1:D:67:GLU:O	2.50	0.45
1:D:11:HIS:HB3	1:D:32:VAL:O	2.17	0.45
1:D:43:ASP:OD2	1:D:45:ASN:N	2.49	0.45
1:D:380:TYR:CE1	1:D:382:PRO:HD3	2.52	0.45
1:B:53:ASN:ND2	1:B:195:SER:O	2.50	0.44
1:B:408:GLN:HG3	1:B:409:PHE:N	2.29	0.44
1:A:44:ASP:OD1	1:A:45:ASN:ND2	2.50	0.44
1:A:117:TYR:OH	1:A:168:GLY:HA2	2.16	0.44
1:A:221:TYR:O	1:A:222:ALA:HB2	2.18	0.44
1:B:192:TRP:CZ2	1:B:202:GLY:HA3	2.52	0.44
1:B:216:TRP:NE1	1:B:218:SER:OG	2.50	0.44
1:C:65:CYS:HB2	1:C:187:ALA:HB2	1.98	0.44
1:C:345:VAL:O	1:C:350:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:O	1:A:413:GLN:HA	2.18	0.44
1:A:189:ILE:O	1:A:192:TRP:N	2.50	0.44
1:A:272:ASP:OD1	1:A:272:ASP:N	2.50	0.44
1:A:384:LYS:O	1:A:385:GLU:HB3	2.16	0.44
1:A:402:PRO:HB2	2:A:478:HOH:O	2.17	0.44
1:B:2:ARG:NH2	1:B:67:GLU:O	2.49	0.44
1:B:122:LEU:HD22	1:B:359:MET:CG	2.47	0.44
1:D:1:PCA:HA	1:D:66:ALA:O	2.18	0.44
1:A:3:ALA:HB1	1:A:167:TYR:HH	1.79	0.44
1:A:363:MET:HE2	1:A:363:MET:HB2	1.62	0.44
1:B:12:PRO:HA	1:B:13:PRO:HD3	1.89	0.44
1:B:135:THR:O	1:B:412:ALA:HA	2.18	0.44
1:C:41:LEU:HD11	1:C:71:ILE:HD11	1.99	0.44
1:C:244:GLY:HA2	1:C:250:ASP:O	2.18	0.44
1:A:312:PRO:HG2	1:A:320:ASN:HD21	1.82	0.44
1:B:81:TYR:C	1:B:96:THR:HG21	2.43	0.44
1:B:198:ASP:HB3	1:B:201:ALA:CB	2.47	0.44
1:B:222:ALA:HB3	1:B:376:LEU:O	2.17	0.44
1:B:341:ARG:O	1:B:344:GLU:N	2.50	0.44
1:C:257:ASP:HA	1:C:341:ARG:HG3	1.98	0.44
1:A:414:VAL:HG11	1:A:416:TRP:NE1	2.32	0.44
1:B:266:TYR:OH	1:B:394:ASP:OD1	2.29	0.44
1:B:267:ARG:HD3	1:B:336:PHE:HE2	1.83	0.44
1:C:98:HIS:HB2	1:C:101:GLY:CA	2.47	0.44
1:C:380:TYR:CG	1:C:381:PRO:HA	2.52	0.44
1:A:5:ASN:N	1:A:72:GLU:OE2	2.50	0.44
1:A:268:MET:SD	1:A:318:MET:HE1	2.57	0.44
1:A:384:LYS:HD2	1:A:384:LYS:HA	1.76	0.44
1:B:42:HIS:ND1	1:B:43:ASP:O	2.50	0.44
1:B:61:THR:N	1:B:64:ASP:OD2	2.50	0.44
1:C:16:TRP:HB2	1:C:419:ILE:HB	1.99	0.44
1:C:306:ARG:NH1	1:D:130:ASP:OD2	2.50	0.44
1:D:207:GLY:HA3	1:D:238:CYS:SG	2.57	0.44
1:A:348:PHE:O	1:A:352:ASN:N	2.50	0.44
1:B:341:ARG:NE	2:B:434:HOH:O	2.50	0.44
1:C:48:ASN:ND2	1:C:51:ASP:OD1	2.50	0.44
1:C:373:MET:HG3	1:C:376:LEU:HB3	2.00	0.44
1:A:341:ARG:O	1:A:344:GLU:N	2.50	0.44
1:B:9:GLU:CD	1:B:39:ARG:HH22	2.26	0.44
1:C:306:ARG:HH12	1:D:418:ASN:HD22	1.66	0.44
1:D:297:LEU:HD11	1:D:355:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:SER:CB	1:B:201:ALA:HB3	2.48	0.43
1:B:332:MET:HE3	1:B:332:MET:HB3	1.89	0.43
1:C:41:LEU:CD2	1:C:71:ILE:HG12	2.48	0.43
1:D:144:LEU:HD21	1:D:361:LEU:HD11	2.00	0.43
1:A:273:PHE:CD1	1:A:279:THR:HB	2.53	0.43
1:B:383:GLU:H	1:B:383:GLU:HG2	1.24	0.43
1:C:349:GLU:OE2	1:C:352:ASN:HB2	2.18	0.43
1:A:141:ASN:HB2	1:A:373:MET:SD	2.58	0.43
1:A:188:ASN:HB3	1:A:192:TRP:CZ3	2.53	0.43
1:C:295:ASN:HA	1:C:348:PHE:CE2	2.53	0.43
1:A:53:ASN:O	1:A:54:GLN:HG2	2.19	0.43
1:B:352:ASN:O	1:B:356:ARG:HG3	2.19	0.43
1:C:41:LEU:CG	1:C:71:ILE:HG12	2.46	0.43
1:C:42:HIS:CE1	1:C:46:MET:HE3	2.54	0.43
1:C:49:CYS:HA	1:C:58:ALA:HB3	1.99	0.43
1:C:57:ASN:ND2	2:C:606:HOH:O	2.50	0.43
1:A:30:ALA:O	1:A:31:GLU:HB3	2.18	0.43
1:B:38:TRP:CE2	1:B:106:SER:HA	2.54	0.43
1:B:103:ASN:OD1	1:B:104:VAL:N	2.52	0.43
1:C:64:ASP:OD1	1:C:68:LYS:NZ	2.50	0.43
1:D:109:TYR:CD1	1:D:362:VAL:HG22	2.53	0.43
1:D:213:ILE:N	1:D:213:ILE:HD12	2.34	0.43
1:A:332:MET:HE3	1:A:336:PHE:HE2	1.84	0.43
1:B:14:LEU:HD12	1:B:14:LEU:HA	1.75	0.43
1:B:96:THR:CG2	1:B:103:ASN:HB3	2.49	0.43
1:B:182:PHE:HB2	2:B:563:HOH:O	2.19	0.43
1:B:310:ILE:O	1:B:322:SER:HB3	2.19	0.43
1:C:34:ILE:HB	1:C:108:PHE:CE2	2.53	0.43
1:C:147:VAL:HG23	1:C:149:MET:HG3	2.00	0.43
1:A:164:GLY:O	1:A:169:THR:HG23	2.18	0.43
1:A:404:GLU:O	1:A:408:GLN:HB3	2.19	0.43
1:B:155:MET:CE	1:B:166:ARG:HD2	2.49	0.43
1:A:4:GLY:HA2	1:A:70:MET:HE3	2.00	0.43
1:A:395:CYS:HA	1:A:396:PRO:HD3	1.85	0.43
1:B:97:LYS:HB3	1:B:102:THR:OG1	2.17	0.43
1:B:144:LEU:CD2	1:B:361:LEU:HD11	2.45	0.43
1:B:296:LYS:HE3	2:B:504:HOH:O	2.19	0.43
1:C:44:ASP:HA	1:C:70:MET:HE1	1.99	0.43
1:D:79:GLY:O	1:D:98:HIS:HB3	2.19	0.43
1:B:53:ASN:OD1	1:B:53:ASN:N	2.51	0.43
1:C:389:GLY:HA3	2:C:507:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ASN:HD21	1:C:420:ARG:HH21	1.66	0.43
1:D:78:LEU:HG	1:D:84:SER:HB3	1.99	0.43
1:B:264:ASN:OD1	1:B:266:TYR:N	2.49	0.43
1:B:397:THR:OG1	1:B:398:ASP:N	2.50	0.43
1:C:61:THR:HG1	1:C:64:ASP:H	1.66	0.43
1:A:161:ASN:OD1	1:A:164:GLY:N	2.49	0.42
1:A:329:CYS:SG	1:A:348:PHE:HE1	2.42	0.42
1:A:363:MET:HG2	1:A:416:TRP:CG	2.54	0.42
1:B:76:ASP:CB	1:C:76:ASP:HA	2.46	0.42
1:D:123:MET:HE3	1:D:356:ARG:HD2	1.99	0.42
1:A:36:ALA:HA	1:A:39:ARG:HG3	2.00	0.42
1:A:297:LEU:HD11	1:A:355:LEU:HD11	2.01	0.42
1:B:231:THR:HG22	1:B:345:VAL:O	2.19	0.42
1:B:295:ASN:ND2	1:B:326:PRO:HG2	2.34	0.42
1:A:178:ARG:CG	1:A:247:TYR:HB2	2.46	0.42
1:B:4:GLY:HA3	1:B:71:ILE:O	2.20	0.42
1:B:152:ASP:O	1:B:155:MET:HG3	2.19	0.42
1:C:39:ARG:HD3	1:C:72:GLU:O	2.19	0.42
1:D:2:ARG:O	1:D:70:MET:HA	2.19	0.42
1:D:43:ASP:OD1	1:D:47:GLN:N	2.50	0.42
1:B:6:GLU:HB2	1:B:72:GLU:CD	2.45	0.42
1:C:53:ASN:CG	1:C:194:SER:HB3	2.44	0.42
1:D:59:CYS:CB	1:D:65:CYS:HG	2.27	0.42
1:D:348:PHE:CZ	1:D:351:LEU:HD23	2.54	0.42
1:A:139:GLY:HA2	1:A:400:GLY:HA2	2.01	0.42
1:B:257:ASP:OD1	1:B:259:ASN:HB3	2.19	0.42
1:B:293:GLU:OE1	1:B:424:ILE:HD13	2.20	0.42
1:C:277:GLY:HA2	1:C:281:ASP:OD2	2.19	0.42
1:D:334:ASP:HB2	1:D:335:VAL:H	1.64	0.42
1:A:280:LEU:HD22	1:A:280:LEU:HA	1.87	0.42
1:B:36:ALA:O	1:B:39:ARG:N	2.50	0.42
1:B:198:ASP:HB2	1:B:369:HIS:CE1	2.54	0.42
1:C:136:VAL:HG12	1:C:219:ASN:CB	2.50	0.42
1:A:219:ASN:ND2	1:A:221:TYR:HD1	2.18	0.42
1:A:257:ASP:OD1	1:A:341:ARG:HB3	2.19	0.42
1:B:149:MET:HB2	1:B:360:VAL:CG2	2.49	0.42
1:B:234:GLU:H	1:B:234:GLU:HG2	1.22	0.42
1:C:272:ASP:OD1	1:C:278:LYS:NZ	2.49	0.42
1:D:9:GLU:OE1	1:D:77:TYR:OH	2.33	0.42
1:A:221:TYR:CE1	1:A:276:LYS:HE3	2.55	0.42
1:A:229:ALA:HB2	1:A:351:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLU:N	1:B:72:GLU:OE2	2.49	0.42
1:B:122:LEU:HD22	1:B:359:MET:SD	2.60	0.42
1:D:119:MET:HE3	1:D:119:MET:HB3	1.90	0.42
1:D:176:CYS:HA	1:D:208:SER:O	2.20	0.42
1:A:132:ASP:HB3	1:A:415:VAL:CG2	2.50	0.42
1:B:76:ASP:OD2	1:B:76:ASP:O	2.37	0.42
1:B:412:ALA:O	1:B:413:GLN:HB3	2.20	0.42
1:B:77:TYR:O	1:B:81:TYR:HB2	2.19	0.42
1:B:178:ARG:O	1:B:203:VAL:HA	2.20	0.42
1:B:195:SER:HB2	1:B:201:ALA:HB3	2.01	0.42
1:B:270:ASN:ND2	1:B:311:PRO:HB2	2.34	0.42
1:B:300:TYR:CG	1:B:307:LYS:HE3	2.54	0.42
1:C:405:VAL:HA	1:C:408:GLN:CG	2.49	0.42
1:A:36:ALA:O	1:A:39:ARG:HG3	2.20	0.41
1:B:196:THR:N	2:B:570:HOH:O	2.52	0.41
1:B:269:GLY:C	1:B:271:PRO:HD3	2.45	0.41
1:C:40:TRP:CE3	1:C:72:GLU:HG3	2.55	0.41
1:C:96:THR:HG23	2:C:550:HOH:O	2.19	0.41
1:B:1:PCA:N	1:B:161:ASN:HA	2.35	0.41
1:B:26:GLN:H	1:B:26:GLN:HG3	1.64	0.41
1:B:147:VAL:HG13	1:B:212:GLU:HG3	2.02	0.41
1:B:289:VAL:HG21	1:B:300:TYR:CE1	2.55	0.41
1:C:187:ALA:HB3	1:C:189:ILE:HG22	2.01	0.41
1:B:83:ALA:HA	1:B:91:THR:O	2.20	0.41
1:B:193:LYS:HD2	1:B:193:LYS:HA	1.69	0.41
1:B:295:ASN:O	1:B:325:THR:HG22	2.20	0.41
1:C:402:PRO:HA	1:C:405:VAL:HG22	2.01	0.41
1:B:155:MET:HE2	1:B:164:GLY:CA	2.42	0.41
1:C:141:ASN:HB2	1:C:373:MET:HE3	2.01	0.41
1:D:310:ILE:HA	1:D:311:PRO:HD3	1.96	0.41
1:A:82:GLY:CA	1:A:96:THR:HG21	2.51	0.41
1:A:96:THR:O	1:A:102:THR:HA	2.19	0.41
1:A:266:TYR:HB3	1:A:392:ARG:O	2.21	0.41
1:B:53:ASN:HB2	1:B:194:SER:OG	2.20	0.41
1:C:65:CYS:HB2	1:C:187:ALA:CB	2.51	0.41
1:C:215:VAL:HA	1:C:225:PHE:CE2	2.56	0.41
1:A:14:LEU:HD12	1:A:85:THR:OG1	2.21	0.41
1:A:155:MET:HE1	1:A:166:ARG:HE	1.84	0.41
1:A:374:LEU:HD23	1:A:378:SER:HB3	2.01	0.41
1:B:55:TRP:NE1	1:B:189:ILE:HA	2.36	0.41
1:B:83:ALA:HB2	1:B:92:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:GLY:HA2	1:B:373:MET:CB	2.50	0.41
1:C:1:PCA:HB2	1:C:71:ILE:HG13	2.01	0.41
1:A:182:PHE:HA	1:A:186:LYS:O	2.21	0.41
1:A:208:SER:HB2	1:A:235:TYR:HE1	1.81	0.41
1:A:263:TYR:CE1	1:A:322:SER:HA	2.55	0.41
1:A:295:ASN:HA	1:A:348:PHE:CD2	2.56	0.41
1:B:126:GLU:HA	1:B:290:SER:O	2.20	0.41
1:B:144:LEU:HG	1:B:362:VAL:O	2.20	0.41
1:B:195:SER:HB3	1:B:198:ASP:O	2.20	0.41
1:B:266:TYR:CE2	1:B:271:PRO:HB3	2.55	0.41
1:D:212:GLU:OE2	1:D:214:ASP:OD1	2.38	0.41
1:A:152:ASP:OD2	1:A:156:ALA:N	2.53	0.41
1:A:414:VAL:HG11	1:A:416:TRP:CE2	2.56	0.41
1:B:114:PRO:O	1:B:166:ARG:HB3	2.20	0.41
1:B:357:VAL:O	1:B:359:MET:HE2	2.21	0.41
1:B:379:ILE:HD12	1:B:379:ILE:N	2.36	0.41
1:C:294:GLU:O	1:C:294:GLU:HG2	2.21	0.41
1:C:377:ASP:O	1:C:395:CYS:HB2	2.20	0.41
1:A:55:TRP:CD1	1:A:55:TRP:H	2.38	0.41
1:A:127:LEU:HB2	1:A:421:PHE:HD1	1.86	0.41
1:A:147:VAL:CG1	1:A:212:GLU:HG3	2.50	0.41
1:A:252:PHE:HE2	1:A:259:ASN:ND2	2.18	0.41
1:A:266:TYR:N	2:A:541:HOH:O	2.53	0.41
1:B:123:MET:HE2	1:B:356:ARG:NH2	2.36	0.41
1:D:361:LEU:HD12	1:D:362:VAL:N	2.35	0.41
1:B:71:ILE:HD13	1:B:71:ILE:HG21	1.86	0.41
1:C:76:ASP:CG	1:C:79:GLY:H	2.28	0.41
1:C:263:TYR:CE1	1:C:322:SER:HA	2.56	0.41
1:A:223:PHE:CZ	1:A:301:PHE:HZ	2.39	0.40
1:A:341:ARG:O	1:A:341:ARG:HG3	2.20	0.40
1:B:175:GLN:HG3	1:B:258:ALA:CB	2.46	0.40
1:B:243:CYS:O	1:B:253:ALA:HB3	2.20	0.40
1:C:98:HIS:ND1	1:C:102:THR:N	2.69	0.40
1:D:381:PRO:HA	1:D:382:PRO:HD3	1.87	0.40
1:A:4:GLY:HA3	1:A:72:GLU:CD	2.46	0.40
1:A:149:MET:HE3	1:A:171:TYR:N	2.36	0.40
1:A:367:ASP:OD1	1:A:367:ASP:N	2.50	0.40
1:C:268:MET:HB2	2:C:600:HOH:O	2.20	0.40
1:D:125:ASN:ND2	2:D:598:HOH:O	2.49	0.40
1:A:116:LYS:NZ	2:A:451:HOH:O	2.50	0.40
1:B:53:ASN:ND2	1:B:194:SER:HB3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LYS:HA	1:B:413:GLN:HB3	2.03	0.40
1:B:111:MET:HA	1:B:118:GLN:H	1.87	0.40
1:B:284:ARG:HB3	1:B:303:GLN:NE2	2.36	0.40
1:B:291:ARG:HB3	1:B:424:ILE:CG1	2.51	0.40
1:C:265:PRO:HA	2:C:600:HOH:O	2.20	0.40
1:D:139:GLY:HA3	1:D:400:GLY:HA2	2.03	0.40
1:D:383:GLU:OE2	1:D:383:GLU:HA	2.21	0.40
1:B:143:ALA:CB	1:B:366:TRP:HE1	2.33	0.40
1:B:175:GLN:OE1	1:B:258:ALA:HA	2.22	0.40
1:D:41:LEU:HD22	1:D:69:CYS:CB	2.51	0.40
1:A:178:ARG:HG3	1:A:247:TYR:CB	2.48	0.40
1:A:356:ARG:CB	1:B:24:ASN:HD21	2.33	0.40
1:B:127:LEU:HD22	1:B:146:PHE:CZ	2.56	0.40
1:B:349:GLU:O	1:B:352:ASN:N	2.54	0.40
1:D:307:LYS:HE3	1:D:430:PHE:O	2.20	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	428/430 (100%)	356 (83%)	52 (12%)	20 (5%)	2	0
1	B	428/430 (100%)	356 (83%)	57 (13%)	15 (4%)	3	0
1	C	428/430 (100%)	409 (96%)	15 (4%)	4 (1%)	14	3
1	D	428/430 (100%)	398 (93%)	24 (6%)	6 (1%)	9	1
All	All	1712/1720 (100%)	1519 (89%)	148 (9%)	45 (3%)	4	0

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ALA
1	A	190	GLU
1	A	240	THR
1	A	337	ASN
1	A	399	SER
1	B	4	GLY
1	B	24	ASN
1	B	29	ASN
1	B	46	MET
1	B	429	ASP
1	C	384	LYS
1	D	99	GLU
1	D	385	GLU
1	A	60	SER
1	A	189	ILE
1	A	210	CYS
1	A	339	ARG
1	A	385	GLU
1	B	23	GLY
1	B	196	THR
1	B	210	CYS
1	B	296	LYS
1	B	385	GLU
1	C	240	THR
1	D	334	ASP
1	D	382	PRO
1	A	94	PHE
1	A	402	PRO
1	B	214	ASP
1	B	418	ASN
1	C	98	HIS
1	C	176	CYS
1	A	31	GLU
1	A	43	ASP
1	A	328	LEU
1	A	429	ASP
1	B	249	GLU
1	D	176	CYS
1	A	148	ALA
1	B	176	CYS
1	B	384	LYS
1	D	87	GLY
1	A	79	GLY

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Mol	Chain	Res	Type
1	A	338	ASP
1	A	105	GLY

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	354/354 (100%)	277 (78%)	77 (22%)	1 0
1	B	354/354 (100%)	266 (75%)	88 (25%)	0 0
1	C	354/354 (100%)	320 (90%)	34 (10%)	8 1
1	D	354/354 (100%)	325 (92%)	29 (8%)	10 2
All	All	1416/1416 (100%)	1188 (84%)	228 (16%)	2 0

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	14	LEU
1	A	17	GLN
1	A	18	ARG
1	A	27	THR
1	A	45	ASN
1	A	46	MET
1	A	54	GLN
1	A	57	ASN
1	A	59	CYS
1	A	60	SER
1	A	61	THR
1	A	67	GLU
1	A	68	LYS
1	A	71	ILE
1	A	76	ASP
1	A	78	LEU
1	A	84	SER
1	A	85	THR

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Mol	Chain	Res	Type
1	A	86	SER
1	A	96	THR
1	A	97	LYS
1	A	102	THR
1	A	103	ASN
1	A	116	LYS
1	A	119	MET
1	A	127	LEU
1	A	136	VAL
1	A	140	ILE
1	A	162	GLN
1	A	166	ARG
1	A	167	TYR
1	A	175	GLN
1	A	178	ARG
1	A	189	ILE
1	A	196	THR
1	A	198	ASP
1	A	213	ILE
1	A	217	GLU
1	A	234	GLU
1	A	239	GLU
1	A	240	THR
1	A	241	THR
1	A	246	THR
1	A	251	ARG
1	A	270	ASN
1	A	272	ASP
1	A	276	LYS
1	A	280	LEU
1	A	284	ARG
1	A	285	LYS
1	A	288	VAL
1	A	289	VAL
1	A	290	SER
1	A	292	PHE
1	A	296	LYS
1	A	297	LEU
1	A	298	SER
1	A	308	ILE
1	A	309	GLU
1	A	318	MET

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Mol	Chain	Res	Type
1	A	322	SER
1	A	328	LEU
1	A	330	SER
1	A	334	ASP
1	A	338	ASP
1	A	343	GLU
1	A	361	LEU
1	A	362	VAL
1	A	363	MET
1	A	383	GLU
1	A	384	LYS
1	A	404	GLU
1	A	408	GLN
1	A	411	ASP
1	A	420	ARG
1	A	424	ILE
1	B	5	ASN
1	B	15	THR
1	B	18	ARG
1	B	20	THR
1	B	26	GLN
1	B	27	THR
1	B	28	VAL
1	B	29	ASN
1	B	34	ILE
1	B	37	ASN
1	B	51	ASP
1	B	53	ASN
1	B	54	GLN
1	B	59	CYS
1	B	61	THR
1	B	68	LYS
1	B	71	ILE
1	B	76	ASP
1	B	78	LEU
1	B	80	THR
1	B	85	THR
1	B	86	SER
1	B	91	THR
1	B	92	LEU
1	B	93	LYS
1	B	95	VAL

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Mol	Chain	Res	Type
1	B	96	THR
1	B	104	VAL
1	B	110	LEU
1	B	116	LYS
1	B	121	ASN
1	B	122	LEU
1	B	123	MET
1	B	126	GLU
1	B	142	SER
1	B	147	VAL
1	B	155	MET
1	B	162	GLN
1	B	166	ARG
1	B	175	GLN
1	B	181	LYS
1	B	183	VAL
1	B	186	LYS
1	B	189	ILE
1	B	190	GLU
1	B	193	LYS
1	B	194	SER
1	B	196	THR
1	B	200	ASN
1	B	203	VAL
1	B	208	SER
1	B	214	ASP
1	B	218	SER
1	B	219	ASN
1	B	234	GLU
1	B	242	ASN
1	B	251	ARG
1	B	267	ARG
1	B	285	LYS
1	B	289	VAL
1	B	293	GLU
1	B	294	GLU
1	B	296	LYS
1	B	297	LEU
1	B	298	SER
1	B	302	ILE
1	B	306	ARG
1	B	310	ILE

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Mol	Chain	Res	Type
1	B	316	GLU
1	B	321	SER
1	B	328	LEU
1	B	332	MET
1	B	335	VAL
1	B	345	VAL
1	B	356	ARG
1	B	359	MET
1	B	365	ILE
1	B	369	HIS
1	B	373	MET
1	B	376	LEU
1	B	383	GLU
1	B	384	LYS
1	B	385	GLU
1	B	392	ARG
1	B	398	ASP
1	B	405	VAL
1	B	409	PHE
1	B	424	ILE
1	C	20	THR
1	C	26	GLN
1	C	32	VAL
1	C	39	ARG
1	C	41	LEU
1	C	43	ASP
1	C	45	ASN
1	C	51	ASP
1	C	54	GLN
1	C	63	THR
1	C	64	ASP
1	C	71	ILE
1	C	78	LEU
1	C	96	THR
1	C	100	TYR
1	C	115	ASP
1	C	122	LEU
1	C	189	ILE
1	C	190	GLU
1	C	193	LYS
1	C	234	GLU
1	C	276	LYS

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Mol	Chain	Res	Type
1	C	281	ASP
1	C	285	LYS
1	C	294	GLU
1	C	296	LYS
1	C	328	LEU
1	C	330	SER
1	C	349	GLU
1	C	350	GLN
1	C	385	GLU
1	C	394	ASP
1	C	415	VAL
1	C	419	ILE
1	D	2	ARG
1	D	5	ASN
1	D	18	ARG
1	D	37	ASN
1	D	41	LEU
1	D	51	ASP
1	D	57	ASN
1	D	60	SER
1	D	71	ILE
1	D	76	ASP
1	D	78	LEU
1	D	93	LYS
1	D	97	LYS
1	D	115	ASP
1	D	122	LEU
1	D	155	MET
1	D	181	LYS
1	D	190	GLU
1	D	234	GLU
1	D	246	THR
1	D	284	ARG
1	D	285	LYS
1	D	332	MET
1	D	356	ARG
1	D	365	ILE
1	D	384	LYS
1	D	385	GLU
1	D	398	ASP
1	D	424	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	24	ASN
1	A	26	GLN
1	A	29	ASN
1	A	42	HIS
1	A	54	GLN
1	A	125	ASN
1	A	175	GLN
1	A	270	ASN
1	A	320	ASN
1	A	340	ASN
1	A	352	ASN
1	A	369	HIS
1	A	387	GLN
1	A	408	GLN
1	B	5	ASN
1	B	24	ASN
1	B	29	ASN
1	B	162	GLN
1	B	200	ASN
1	B	320	ASN
1	B	340	ASN
1	B	350	GLN
1	B	352	ASN
1	B	369	HIS
1	B	372	ASN
1	B	418	ASN
1	C	29	ASN
1	C	125	ASN
1	C	200	ASN
1	C	320	ASN
1	C	340	ASN
1	C	352	ASN
1	C	353	ASN
1	C	369	HIS
1	C	387	GLN
1	D	45	ASN
1	D	121	ASN
1	D	125	ASN
1	D	242	ASN
1	D	320	ASN
1	D	340	ASN

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Mol	Chain	Res	Type
1	D	352	ASN
1	D	353	ASN
1	D	369	HIS
1	D	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PCA	B	1	1	7,8,9	2.22	1 (14%)	9,10,12	1.74	4 (44%)
1	PCA	A	1	1	7,8,9	2.11	1 (14%)	9,10,12	1.59	2 (22%)
1	PCA	C	1	1	7,8,9	2.06	1 (14%)	9,10,12	1.53	2 (22%)
1	PCA	D	1	1	7,8,9	1.98	1 (14%)	9,10,12	1.34	1 (11%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	PCA	CD-N	5.48	1.48	1.34
1	A	1	PCA	CD-N	5.14	1.47	1.34
1	C	1	PCA	CD-N	4.97	1.46	1.34
1	D	1	PCA	CD-N	4.89	1.46	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	PCA	CB-CA-C	-3.03	108.50	112.66
1	B	1	PCA	CB-CG-CD	2.95	108.97	104.41
1	B	1	PCA	OE-CD-CG	-2.66	121.97	126.72
1	C	1	PCA	OE-CD-CG	-2.64	122.01	126.72
1	A	1	PCA	CB-CA-C	-2.54	109.17	112.66
1	A	1	PCA	CB-CG-CD	2.36	108.07	104.41
1	C	1	PCA	CB-CG-CD	2.29	107.96	104.41
1	B	1	PCA	CB-CA-C	-2.04	109.86	112.66
1	B	1	PCA	CG-CD-N	-2.02	103.44	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	PCA	1	0
1	A	1	PCA	1	0
1	C	1	PCA	1	0
1	D	1	PCA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [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	429/430 (99%)	-0.29	0 100 100	14, 27, 42, 58	0
1	B	429/430 (99%)	-0.23	0 100 100	13, 28, 44, 70	0
1	C	429/430 (99%)	-0.90	0 100 100	5, 13, 28, 62	0
1	D	429/430 (99%)	-0.99	0 100 100	4, 12, 26, 62	0
All	All	1716/1720 (99%)	-0.61	0 100 100	4, 21, 40, 70	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	A	1	8/9	0.98	0.07	12,23,30,58	0
1	PCA	B	1	8/9	0.98	0.06	16,28,39,63	0
1	PCA	C	1	8/9	0.99	0.04	13,17,21,21	0
1	PCA	D	1	8/9	0.99	0.03	6,11,19,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.