



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:27 PM UTC

PDB ID : 1QNI / pdb_00001qni
Title : Crystal Structure of Nitrous Oxide Reductase from Pseudomonas nautica, at 2.4Å Resolution
Authors : Brown, K.; Tegoni, M.; Cambillau, C.
Deposited on : 1999-10-15
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

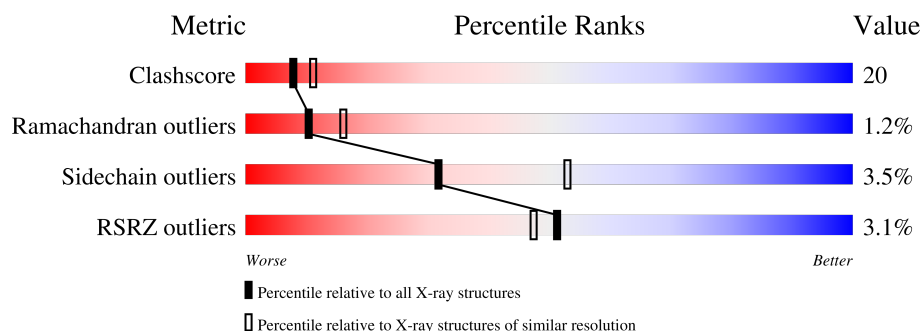
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	581	
1	B	581	
1	C	581	
1	D	581	
1	E	581	
1	F	581	

2 Entry composition [i](#)

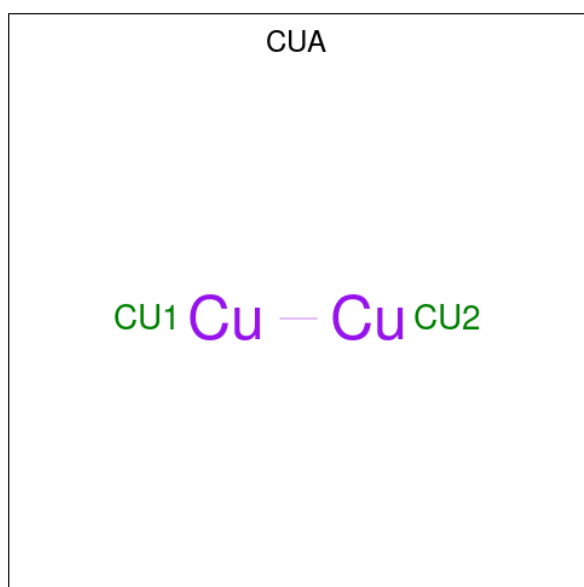
There are 6 unique types of molecules in this entry. The entry contains 28448 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITROUS-OXIDE REDUCTASE.

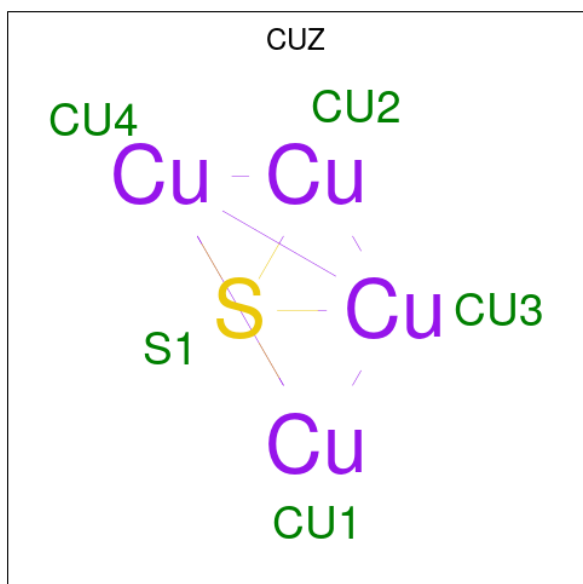
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			
1	B	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			
1	C	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			
1	D	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			
1	E	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			
1	F	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			

- Molecule 2 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 2 2	0	0
2	B	1	Total Cu 2 2	0	0
2	C	1	Total Cu 2 2	0	0
2	D	1	Total Cu 2 2	0	0
2	E	1	Total Cu 2 2	0	0
2	F	1	Total Cu 2 2	0	0

- Molecule 3 is (MU-4-SULFIDO)-TETRA-NUCLEAR COPPER ION (CCD ID: CUZ) (formula: Cu_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu S 5 4 1	0	0
3	B	1	Total Cu S 5 4 1	0	0
3	C	1	Total Cu S 5 4 1	0	0
3	D	1	Total Cu S 5 4 1	0	0
3	E	1	Total Cu S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	Cu	S	0	0
			5	4	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		
4	D	2	Total	Ca	0	0
			2	2		
4	E	2	Total	Ca	0	0
			2	2		
4	F	2	Total	Ca	0	0
			2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	E	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	332	Total	O	0	0
			332	332		
6	B	317	Total	O	0	0
			317	317		

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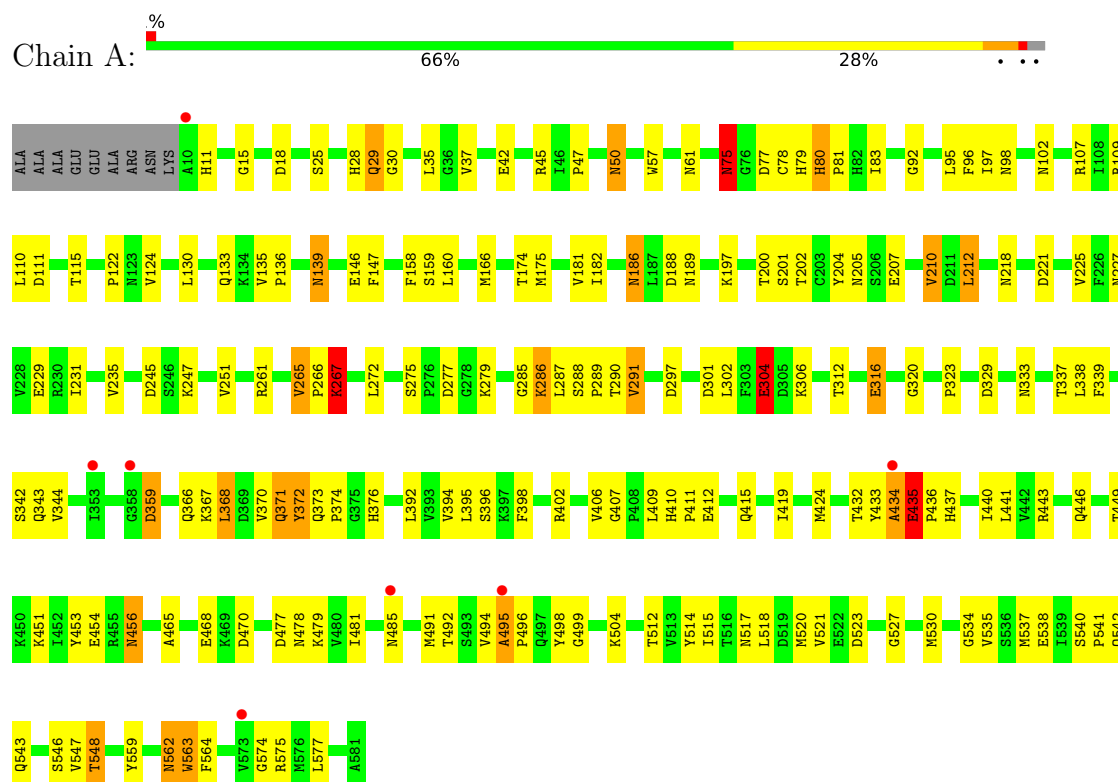
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	97	Total 97	O 97	0	0
6	D	116	Total 116	O 116	0	0
6	E	223	Total 223	O 223	0	0
6	F	225	Total 225	O 225	0	0

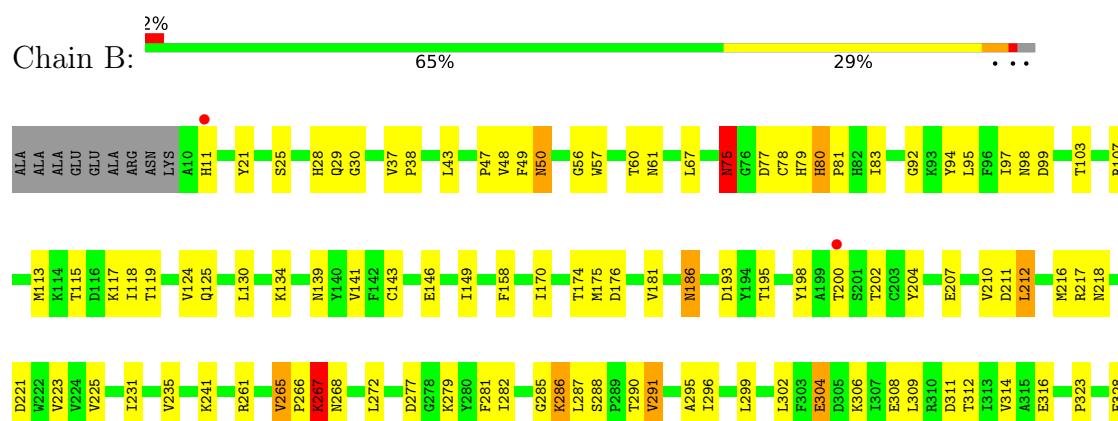
3 Residue-property plots [i](#)

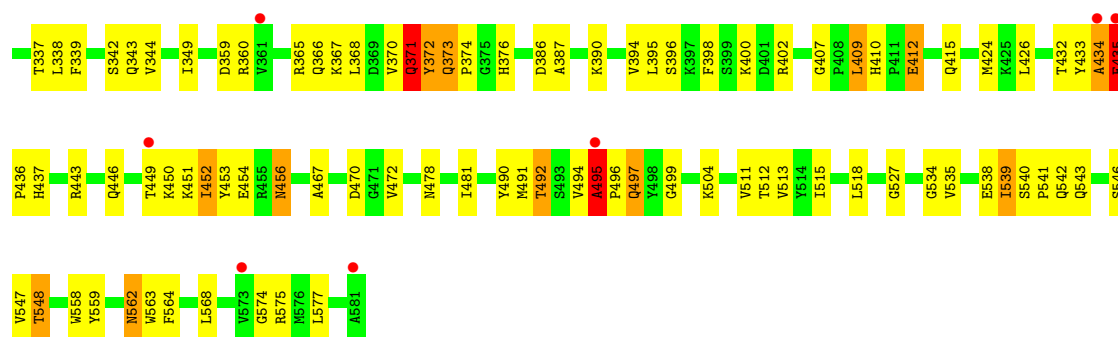
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

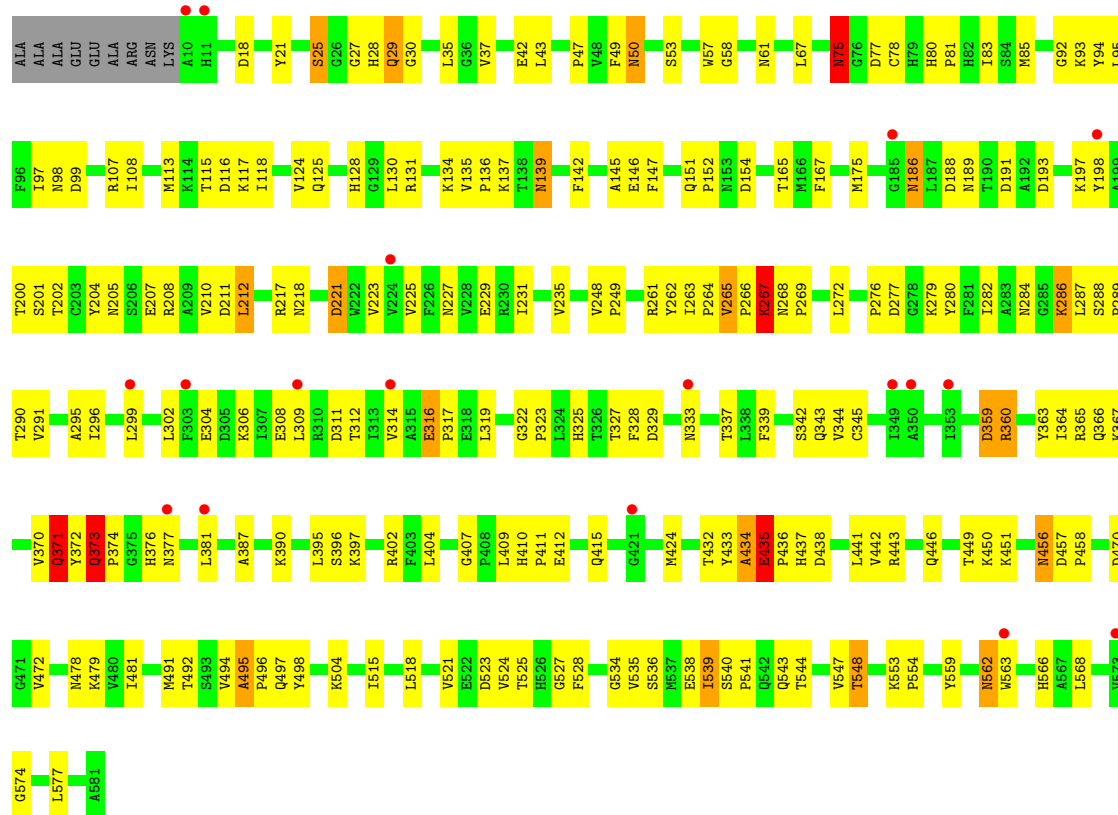


• Molecule 1: NITROUS-OXIDE REDUCTASE

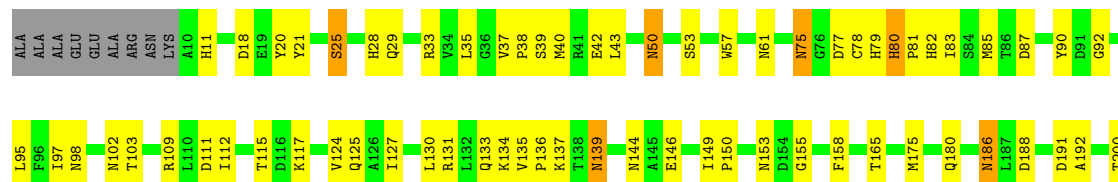


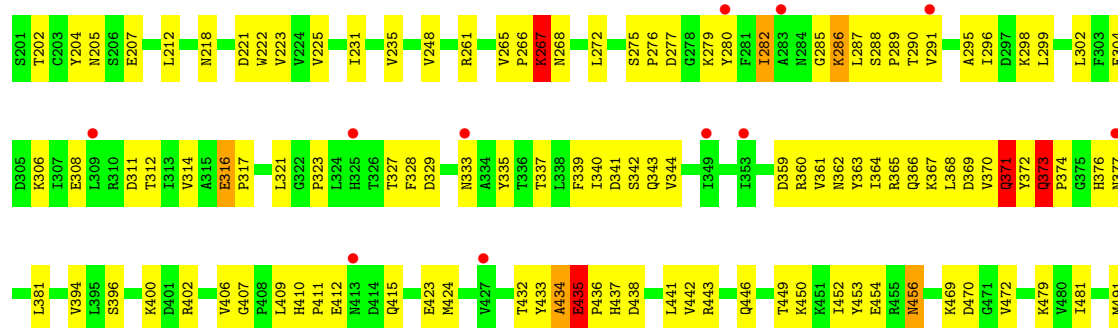


● Molecule 1: NITROUS-OXIDE REDUCTASE

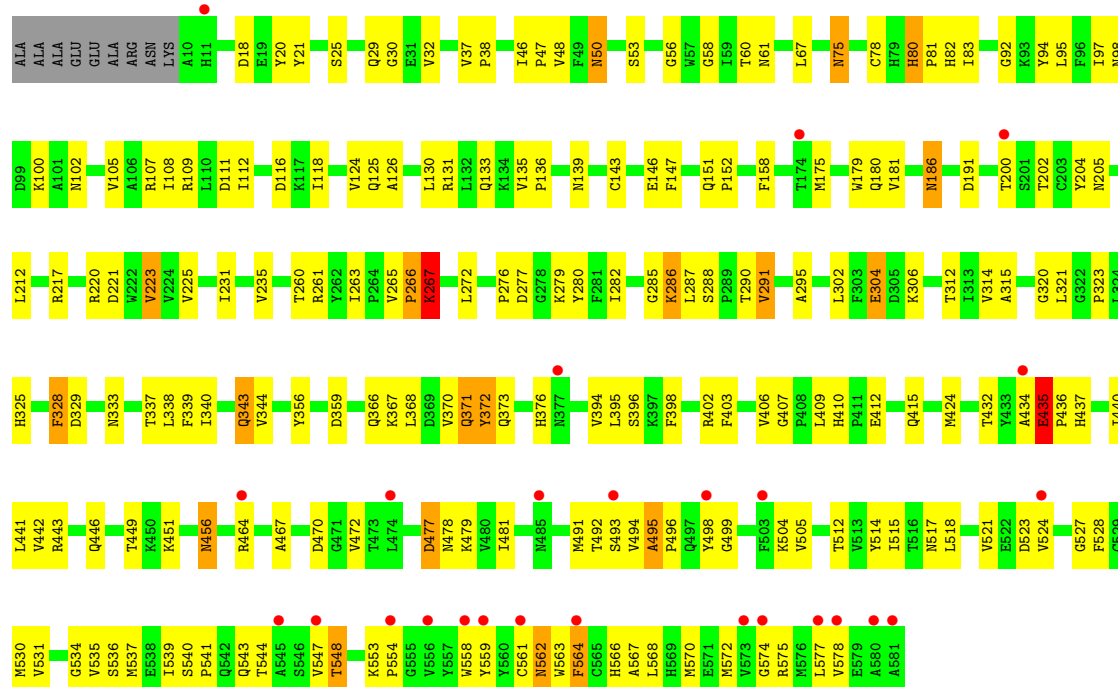


● Molecule 1: NITROUS-OXIDE REDUCTASE

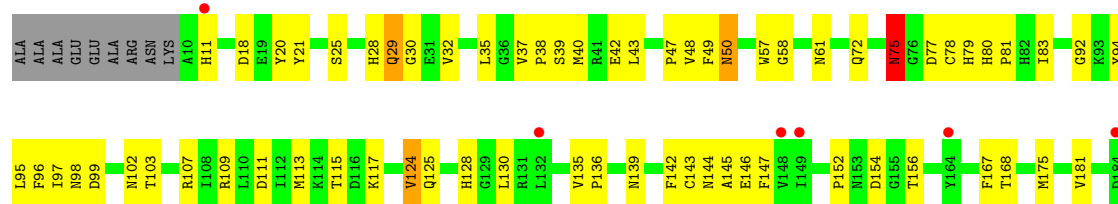




• Molecule 1: NITROUS-OXIDE REDUCTASE



• Molecule 1: NITROUS-OXIDE REDUCTASE



G185	N186	L187	T200	S201	T202	C203	Y204	N205	S206	V210	D211	L212	D221	W222	V223	V224	V225	F226	N227	I231	A232	A233	V248	F259	T260	R261	Y262	I263	P264	V265	P266	K267	N268	P269	H270	G271	L272	S275	P276	D277	G278	K279	Y280	F281	I282	A283	N284	G285	K286	L287	S288	P289
T290	V291	S292	A295	I296	L302	F303	E304	D305	K306	L309	T312	I313	V314	A315	E316	F317	E318	P323	L324	H325	T326	T327	F328	D329	N333	T337	L338	F339	S342	Q343	V344	I353	K354	D359	R360	V361	N362	Y363	I364	K365	Q366	K367	L368	D369	V370	K371	Y372	Q373	S288	P374		
G375	H376	N377	K390	V391	L392	V393	V394	L395	S396	K400	G407	P408	L409	H410	P411	E412	Q415	I419	S420	M424	T432	F433	A434	E435	P436	H437	L440	L441	V442	R443	Q446	T449	K450	K451	I452	Y453	E454	R455	N456	D457	P458	D470	G471	V472	K479	V480	I481					
R482	D483	G484	N485	T492	S493	V494	A495	P496	Q497	Y498	K504	L518	G527	F528	C529	M530	H533	G534	V535	S536	M537	E538	I539	S540	P541	Q542	Q543	V547	T548	H558	Y559	N562	W563	L568	V573	G574	R575	M576	L577	A581												

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	211.29Å 211.29Å 166.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.40) 90.7 (20.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.39Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.228 , 0.261 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28448	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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: CUA, CA, CL, CUZ

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	0.48	0/4619	1.02	24/6271 (0.4%)
1	B	0.48	0/4619	1.03	23/6271 (0.4%)
1	C	0.39	0/4619	0.93	18/6271 (0.3%)
1	D	0.42	0/4619	0.95	15/6271 (0.2%)
1	E	0.46	0/4619	1.01	20/6271 (0.3%)
1	F	0.46	0/4619	0.98	24/6271 (0.4%)
All	All	0.45	0/27714	0.99	124/37626 (0.3%)

There are no bond length outliers.

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	221	ASP	N-CA-C	-9.23	99.89	108.75
1	B	221	ASP	N-CA-C	-8.99	100.12	108.75
1	A	285	GLY	N-CA-C	8.54	124.50	114.16
1	B	285	GLY	N-CA-C	8.33	122.72	112.73
1	A	221	ASP	N-CA-C	-8.29	100.79	108.75
1	B	30	GLY	N-CA-C	7.79	123.96	114.69
1	B	267	LYS	N-CA-C	7.61	127.02	110.80
1	E	146	GLU	N-CA-C	7.53	119.57	111.36
1	E	267	LYS	N-CA-C	7.52	126.82	110.80
1	A	146	GLU	N-CA-C	7.39	121.55	112.23
1	E	30	GLY	N-CA-C	7.37	123.46	114.69
1	E	371	GLN	N-CA-C	7.24	121.57	108.17
1	D	221	ASP	N-CA-C	-7.21	101.83	108.75
1	E	435	GLU	N-CA-C	7.17	125.66	109.81
1	C	221	ASP	N-CA-C	-7.07	101.96	108.75
1	A	435	GLU	N-CA-C	7.07	125.43	109.81
1	F	30	GLY	N-CA-C	6.96	122.97	114.69
1	A	267	LYS	N-CA-C	6.90	125.50	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	146	GLU	N-CA-C	6.86	118.84	111.36
1	F	497	GLN	N-CA-C	6.79	120.59	109.06
1	E	285	GLY	N-CA-C	6.67	122.31	113.37
1	A	30	GLY	N-CA-C	6.65	123.00	115.08
1	A	265	VAL	CA-C-N	6.62	128.12	119.84
1	A	265	VAL	C-N-CA	6.62	128.12	119.84
1	F	29	GLN	N-CA-C	-6.62	104.23	112.90
1	F	75	ASN	N-CA-C	6.58	118.14	108.86
1	B	146	GLU	N-CA-C	6.50	119.69	111.69
1	C	146	GLU	N-CA-C	6.48	118.42	111.36
1	B	435	GLU	N-CA-C	6.47	124.12	109.81
1	A	80	HIS	N-CA-C	6.47	123.29	108.93
1	B	495	ALA	CA-C-N	-6.43	111.81	119.84
1	B	495	ALA	C-N-CA	-6.43	111.81	119.84
1	D	25	SER	N-CA-C	-6.39	102.10	110.53
1	F	435	GLU	N-CA-C	6.39	123.93	109.81
1	C	267	LYS	N-CA-C	6.37	124.36	110.80
1	D	435	GLU	N-CA-C	6.35	123.84	109.81
1	F	267	LYS	N-CA-C	6.34	124.30	110.80
1	C	435	GLU	N-CA-C	6.29	123.72	109.81
1	E	291	VAL	N-CA-C	-6.23	100.12	108.35
1	A	372	TYR	N-CA-C	6.22	124.05	110.80
1	E	223	VAL	N-CA-C	-6.19	99.44	108.11
1	B	139	ASN	N-CA-C	-6.12	105.94	113.41
1	A	29	GLN	N-CA-C	-6.12	104.52	112.23
1	D	285	GLY	N-CA-C	6.11	121.55	114.16
1	B	75	ASN	N-CA-C	6.06	117.41	108.86
1	A	371	GLN	N-CA-C	6.06	119.38	108.17
1	A	139	ASN	N-CA-C	-5.98	105.65	113.12
1	B	497	GLN	N-CA-C	5.97	118.48	109.23
1	D	80	HIS	N-CA-C	5.97	122.17	108.93
1	B	195	THR	N-CA-C	-5.95	107.83	114.62
1	F	285	GLY	N-CA-C	5.93	119.38	112.50
1	B	80	HIS	N-CA-C	5.87	121.16	109.01
1	F	222	TRP	N-CA-C	5.85	116.13	107.88
1	F	485	ASN	N-CA-C	-5.79	106.04	113.23
1	B	281	PHE	N-CA-C	-5.77	99.11	108.52
1	A	498	TYR	N-CA-C	-5.77	101.15	110.32
1	D	371	GLN	N-CA-C	5.75	118.81	108.17
1	B	371	GLN	N-CA-C	5.75	118.52	108.52
1	F	457	ASP	CA-C-N	5.71	125.56	119.28
1	F	457	ASP	C-N-CA	5.71	125.56	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	VAL	CA-C-N	5.66	126.91	119.84
1	B	265	VAL	C-N-CA	5.66	126.91	119.84
1	C	29	GLN	N-CA-C	-5.65	105.88	112.89
1	D	282	ILE	N-CA-C	5.64	115.92	107.51
1	A	304	GLU	N-CA-C	-5.63	105.16	113.61
1	E	32	VAL	N-CA-C	-5.63	100.23	108.11
1	A	454	GLU	N-CA-C	-5.60	100.57	109.76
1	A	75	ASN	N-CA-C	5.60	117.48	109.14
1	F	21	TYR	N-CA-C	-5.57	100.62	109.76
1	F	146	GLU	N-CA-C	5.57	117.16	111.14
1	E	304	GLU	N-CA-C	-5.54	106.42	114.12
1	C	371	GLN	N-CA-C	5.52	118.38	108.17
1	C	280	TYR	N-CA-C	5.51	117.41	108.26
1	E	328	PHE	N-CA-C	5.50	118.19	109.50
1	C	58	GLY	N-CA-C	-5.47	106.98	114.64
1	B	372	TYR	N-CA-C	5.47	122.45	110.80
1	C	30	GLY	N-CA-C	5.43	121.31	114.25
1	F	139	ASN	N-CA-C	-5.39	106.84	113.41
1	B	21	TYR	N-CA-C	-5.38	100.94	109.76
1	C	498	TYR	N-CA-C	-5.38	101.52	110.17
1	F	25	SER	N-CA-C	-5.36	103.45	110.53
1	A	465	ALA	N-CA-C	-5.36	105.48	112.23
1	F	275	SER	CA-C-N	5.33	125.65	119.47
1	F	275	SER	C-N-CA	5.33	125.65	119.47
1	F	372	TYR	N-CA-C	5.33	122.14	110.80
1	F	58	GLY	N-CA-C	-5.29	107.23	114.64
1	B	453	TYR	N-CA-C	5.29	118.31	110.48
1	F	498	TYR	N-CA-C	-5.29	101.91	110.32
1	B	198	TYR	N-CA-C	5.28	118.16	109.72
1	F	573	VAL	N-CA-C	5.27	115.25	108.82
1	C	75	ASN	N-CA-C	5.27	116.29	108.86
1	C	497	GLN	N-CA-C	5.27	117.40	109.23
1	E	263	ILE	N-CA-C	5.27	112.77	107.55
1	A	159	SER	N-CA-C	5.26	117.66	110.24
1	F	371	GLN	N-CA-C	5.25	117.88	108.17
1	C	265	VAL	CA-C-N	5.24	125.54	119.93
1	C	265	VAL	C-N-CA	5.24	125.54	119.93
1	E	147	PHE	N-CA-C	5.22	117.23	108.73
1	B	412	GLU	N-CA-C	-5.21	103.03	110.59
1	C	316	GLU	CA-C-N	5.20	124.96	119.76
1	C	316	GLU	C-N-CA	5.20	124.96	119.76
1	D	316	GLU	CA-C-N	5.19	124.95	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	316	GLU	C-N-CA	5.19	124.95	119.76
1	C	139	ASN	N-CA-C	-5.19	107.12	113.50
1	D	222	TRP	N-CA-C	5.18	114.67	107.73
1	F	145	ALA	N-CA-C	-5.17	100.09	108.52
1	E	477	ASP	N-CA-C	5.16	117.34	110.53
1	E	372	TYR	N-CA-C	5.15	121.76	110.80
1	C	25	SER	N-CA-C	-5.15	103.60	110.55
1	E	266	PRO	N-CA-C	5.14	119.64	111.26
1	E	58	GLY	N-CA-C	-5.13	107.78	113.79
1	D	497	GLN	N-CA-C	5.13	117.53	108.75
1	A	122	PRO	N-CA-C	5.12	120.22	111.68
1	E	280	TYR	N-CA-C	5.11	117.78	109.24
1	E	80	HIS	N-CA-C	5.10	120.06	108.74
1	B	454	GLU	N-CA-C	-5.06	101.47	109.96
1	A	316	GLU	CA-C-N	5.05	124.81	119.76
1	A	316	GLU	C-N-CA	5.05	124.81	119.76
1	D	280	TYR	N-CA-C	5.05	117.30	108.76
1	D	139	ASN	N-CA-C	-5.05	107.25	113.41
1	F	248	VAL	N-CA-C	5.05	113.90	108.95
1	D	267	LYS	N-CA-C	5.02	121.49	110.80
1	A	275	SER	CA-C-N	5.01	124.61	119.05
1	A	275	SER	C-N-CA	5.01	124.61	119.05

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	4513	0	4356	169	0
1	B	4513	0	4356	186	0
1	C	4513	0	4356	192	0
1	D	4513	0	4356	195	0
1	E	4513	0	4356	175	0
1	F	4513	0	4356	198	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	332	0	0	16	0
6	B	317	0	0	16	0
6	C	97	0	0	4	0
6	D	116	0	0	6	0
6	E	223	0	0	14	0
6	F	225	0	0	24	0
All	All	28448	0	26136	1051	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 20.

All (1051) 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:F:83:ILE:HD11	1:F:92:GLY:HA2	1.37	1.01
1:C:83:ILE:HD11	1:C:92:GLY:HA2	1.44	0.99
1:E:443:ARG:H	1:E:446:GLN:HE21	1.09	0.98
1:E:564:PHE:HE2	6:F:2094:HOH:O	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLN:HE22	1:B:424:MET:H	1.02	0.95
1:A:371:GLN:H	1:A:415:GLN:HE22	1.15	0.94
1:C:371:GLN:H	1:C:415:GLN:HE22	1.12	0.94
1:D:371:GLN:H	1:D:415:GLN:HE22	0.94	0.93
1:E:371:GLN:H	1:E:415:GLN:HE22	1.13	0.93
1:B:443:ARG:H	1:B:446:GLN:HE21	1.05	0.92
1:E:564:PHE:CE2	6:F:2094:HOH:O	2.21	0.92
1:D:83:ILE:HD11	1:D:92:GLY:HA2	1.50	0.91
1:D:443:ARG:H	1:D:446:GLN:HE21	0.94	0.90
1:A:75:ASN:HD21	1:B:534:GLY:HA2	1.34	0.89
1:F:443:ARG:H	1:F:446:GLN:HE21	1.16	0.88
1:A:534:GLY:HA2	1:B:75:ASN:HD21	1.36	0.88
1:C:443:ARG:H	1:C:446:GLN:HE21	1.17	0.88
1:D:366:GLN:HE22	1:D:424:MET:H	1.18	0.88
1:E:50:ASN:HD22	1:E:50:ASN:H	1.13	0.88
1:E:200:THR:HG22	1:E:225:VAL:HA	1.57	0.87
1:F:568:LEU:HA	6:F:2218:HOH:O	1.73	0.87
1:A:83:ILE:HD11	1:A:92:GLY:HA2	1.56	0.87
1:F:371:GLN:H	1:F:415:GLN:HE22	1.18	0.87
1:E:366:GLN:HE22	1:E:424:MET:H	1.20	0.86
1:C:535:VAL:HG13	1:C:547:VAL:HG21	1.55	0.86
1:E:75:ASN:HD21	1:F:534:GLY:HA2	1.38	0.86
1:D:371:GLN:H	1:D:415:GLN:NE2	1.74	0.85
1:B:371:GLN:H	1:B:415:GLN:HE22	1.21	0.85
1:E:495:ALA:HB1	1:E:496:PRO:HD2	1.56	0.85
1:A:366:GLN:HE22	1:A:424:MET:H	1.23	0.84
1:B:50:ASN:HD22	1:B:50:ASN:H	1.21	0.84
1:F:50:ASN:H	1:F:50:ASN:HD22	1.25	0.84
1:C:366:GLN:HE22	1:C:424:MET:H	1.24	0.84
1:C:412:GLU:HG3	1:C:435:GLU:HA	1.60	0.83
1:C:495:ALA:HB1	1:C:496:PRO:HD2	1.58	0.83
1:A:50:ASN:H	1:A:50:ASN:HD22	1.23	0.83
1:D:443:ARG:N	1:D:446:GLN:HE21	1.77	0.82
1:A:344:VAL:HG23	1:A:370:VAL:HG21	1.58	0.82
1:B:61:ASN:HD21	1:B:548:THR:HG23	1.41	0.82
1:A:443:ARG:H	1:A:446:GLN:HE21	1.28	0.82
1:C:75:ASN:HD21	1:D:534:GLY:HA2	1.45	0.81
1:D:304:GLU:HG2	1:D:306:LYS:HE2	1.61	0.81
1:F:344:VAL:HG23	1:F:370:VAL:HG21	1.60	0.81
1:D:443:ARG:H	1:D:446:GLN:NE2	1.75	0.80
1:D:495:ALA:HB1	1:D:496:PRO:CD	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ASP:OD1	1:B:279:LYS:HG2	1.82	0.80
1:B:470:ASP:HB3	1:B:481:ILE:HD13	1.62	0.79
1:A:495:ALA:HB1	1:A:496:PRO:CD	2.12	0.79
1:F:61:ASN:HD21	1:F:548:THR:HG22	1.46	0.78
1:E:83:ILE:HD11	1:E:92:GLY:HA2	1.65	0.78
1:D:432:THR:HG21	1:D:436:PRO:HG3	1.64	0.78
1:F:495:ALA:HB1	1:F:496:PRO:CD	2.14	0.78
1:E:535:VAL:HG13	1:E:547:VAL:HG21	1.66	0.77
1:B:495:ALA:HB1	1:B:496:PRO:CD	2.14	0.77
1:D:200:THR:HG22	1:D:225:VAL:HA	1.67	0.77
1:E:75:ASN:ND2	1:F:534:GLY:HA2	1.97	0.77
1:B:83:ILE:HD11	1:B:92:GLY:HA2	1.66	0.77
1:D:535:VAL:HG13	1:D:547:VAL:HG21	1.66	0.77
1:F:80:HIS:H	1:F:98:ASN:ND2	1.82	0.76
1:D:495:ALA:HB1	1:D:496:PRO:HD2	1.66	0.76
1:A:200:THR:HG22	1:A:225:VAL:HA	1.67	0.76
1:C:50:ASN:H	1:C:50:ASN:HD22	1.33	0.76
1:D:527:GLY:HA3	1:D:562:ASN:ND2	2.01	0.75
1:F:568:LEU:HD23	6:F:2218:HOH:O	1.86	0.75
1:F:61:ASN:HD21	1:F:548:THR:CG2	1.99	0.75
1:B:443:ARG:H	1:B:446:GLN:NE2	1.84	0.74
1:C:495:ALA:HB1	1:C:496:PRO:CD	2.17	0.74
1:F:343:GLN:NE2	1:F:367:LYS:HD3	2.03	0.74
1:B:79:HIS:H	1:B:98:ASN:HD21	1.34	0.74
6:A:2297:HOH:O	1:B:211:ASP:HB3	1.87	0.73
1:C:302:LEU:HD11	1:C:309:LEU:HD23	1.70	0.73
1:A:470:ASP:HB3	1:A:481:ILE:HD13	1.71	0.73
1:E:540:SER:H	1:E:543:GLN:HE21	1.37	0.73
1:B:304:GLU:HG2	1:B:306:LYS:HE2	1.71	0.73
1:C:200:THR:HG22	1:C:225:VAL:HA	1.70	0.72
1:C:277:ASP:OD1	1:C:279:LYS:HG2	1.88	0.72
1:B:11:HIS:HA	6:B:2001:HOH:O	1.90	0.72
1:B:67:LEU:HD23	1:B:118:ILE:HD13	1.71	0.72
1:B:366:GLN:HE22	1:B:424:MET:N	1.84	0.72
1:B:443:ARG:HB2	1:B:446:GLN:HG3	1.70	0.72
1:D:527:GLY:HA3	1:D:562:ASN:HD21	1.54	0.72
1:B:267:LYS:HB3	1:B:287:LEU:HB2	1.71	0.72
1:C:344:VAL:HG23	1:C:370:VAL:HG21	1.72	0.72
1:A:75:ASN:ND2	1:B:534:GLY:HA2	2.05	0.72
1:A:495:ALA:HB1	1:A:496:PRO:HD2	1.72	0.72
1:D:75:ASN:HD21	1:D:102:ASN:HD21	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ARG:N	1:B:446:GLN:HE21	1.85	0.71
1:F:443:ARG:N	1:F:446:GLN:HE21	1.88	0.71
1:B:412:GLU:HG3	1:B:435:GLU:HA	1.72	0.71
1:A:540:SER:H	1:A:543:GLN:NE2	1.89	0.70
1:D:75:ASN:ND2	1:D:102:ASN:HD21	1.88	0.70
1:D:412:GLU:HG3	1:D:435:GLU:HA	1.73	0.70
1:E:344:VAL:HG23	1:E:370:VAL:HG21	1.71	0.70
1:E:329:ASP:OD2	1:E:333:ASN:HB2	1.92	0.70
1:A:61:ASN:OD1	1:A:548:THR:HG22	1.92	0.69
1:C:443:ARG:HB2	1:C:446:GLN:HG3	1.74	0.69
1:D:371:GLN:HG2	1:D:402:ARG:HD2	1.74	0.69
1:E:29:GLN:HB2	1:E:434:ALA:CB	2.23	0.69
1:C:504:LYS:HG2	1:C:577:LEU:HB2	1.74	0.69
1:E:223:VAL:HG23	1:E:265:VAL:HG21	1.75	0.69
1:E:456:ASN:HD22	1:E:456:ASN:H	1.39	0.69
1:C:186:ASN:HD21	1:C:204:TYR:H	1.39	0.69
1:B:366:GLN:NE2	1:B:424:MET:H	1.83	0.69
1:F:38:PRO:HB2	6:F:2002:HOH:O	1.93	0.69
1:F:366:GLN:HE22	1:F:424:MET:H	1.38	0.69
1:B:344:VAL:HG23	1:B:370:VAL:HG21	1.74	0.69
1:D:344:VAL:HG23	1:D:370:VAL:HG21	1.74	0.68
1:F:443:ARG:HB2	1:F:446:GLN:HG3	1.75	0.68
1:B:495:ALA:HB1	1:B:496:PRO:HD2	1.74	0.68
1:E:410:HIS:CE1	1:F:451:LYS:HE3	2.28	0.68
1:D:79:HIS:H	1:D:98:ASN:HD21	1.40	0.68
1:A:534:GLY:HA2	1:B:75:ASN:ND2	2.07	0.68
1:A:80:HIS:H	1:A:98:ASN:ND2	1.92	0.68
1:B:29:GLN:HB2	1:B:434:ALA:CB	2.24	0.68
1:F:304:GLU:HG2	1:F:306:LYS:HE2	1.74	0.68
1:A:366:GLN:NE2	1:A:424:MET:H	1.92	0.68
1:E:443:ARG:HB2	1:E:446:GLN:HG3	1.75	0.68
1:C:371:GLN:HG2	1:C:402:ARG:HD2	1.74	0.68
6:A:2290:HOH:O	1:E:477:ASP:HA	1.94	0.68
1:C:559:TYR:CZ	1:C:574:GLY:HA3	2.29	0.68
1:F:83:ILE:HD11	1:F:92:GLY:CA	2.19	0.68
1:E:75:ASN:ND2	1:E:102:ASN:HD21	1.92	0.67
1:F:412:GLU:HG3	1:F:435:GLU:HA	1.76	0.67
1:F:483:ASP:HA	6:F:2177:HOH:O	1.93	0.67
1:D:540:SER:H	1:D:543:GLN:HE21	1.43	0.67
1:E:261:ARG:HG2	1:E:302:LEU:HG	1.75	0.67
1:E:267:LYS:HB3	1:E:287:LEU:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:LYS:HB3	1:F:287:LEU:HB2	1.75	0.67
1:A:443:ARG:HB2	1:A:446:GLN:HG3	1.76	0.67
1:F:450:LYS:HD3	6:F:2151:HOH:O	1.95	0.67
1:C:527:GLY:HA3	1:C:562:ASN:ND2	2.10	0.67
1:F:443:ARG:H	1:F:446:GLN:NE2	1.92	0.67
1:D:504:LYS:HG2	1:D:577:LEU:HB2	1.76	0.67
1:A:517:ASN:HD22	1:A:540:SER:C	2.03	0.67
1:B:80:HIS:H	1:B:98:ASN:ND2	1.93	0.67
1:C:496:PRO:HD3	1:C:566:HIS:CD2	2.30	0.67
1:E:75:ASN:HD21	1:E:102:ASN:HD21	1.43	0.66
1:A:478:ASN:HD21	1:A:492:THR:HG22	1.59	0.66
1:E:50:ASN:H	1:E:50:ASN:ND2	1.86	0.66
1:F:472:VAL:HG12	1:F:479:LYS:HD2	1.77	0.66
1:A:78:CYS:HB2	1:A:97:ILE:CD1	2.25	0.66
1:B:504:LYS:HG2	1:B:577:LEU:HB2	1.76	0.66
1:F:286:LYS:H	1:F:323:PRO:HG2	1.60	0.66
1:D:366:GLN:NE2	1:D:424:MET:H	1.92	0.66
1:D:329:ASP:OD2	1:D:333:ASN:HB2	1.95	0.65
1:E:534:GLY:HA2	1:F:75:ASN:HD21	1.61	0.65
1:D:277:ASP:OD1	1:D:279:LYS:HG2	1.96	0.65
1:E:540:SER:H	1:E:543:GLN:NE2	1.92	0.65
1:C:267:LYS:HB3	1:C:287:LEU:HB2	1.78	0.65
1:B:268:ASN:O	1:B:286:LYS:HE2	1.97	0.65
1:E:304:GLU:HG2	1:E:306:LYS:HE2	1.78	0.65
1:F:540:SER:H	1:F:543:GLN:NE2	1.95	0.65
1:F:453:TYR:CD2	1:F:543:GLN:HB2	2.32	0.64
1:B:48:VAL:H	1:B:50:ASN:ND2	1.95	0.64
1:B:61:ASN:ND2	1:B:548:THR:HG23	2.11	0.64
1:E:495:ALA:HB1	1:E:496:PRO:CD	2.28	0.64
1:F:270:HIS:CE1	3:F:801:CUZ:S1	2.91	0.64
1:A:491:MET:HB2	1:A:515:ILE:HD13	1.79	0.64
1:E:570:MET:HE1	1:F:128:HIS:CE1	2.33	0.64
1:C:456:ASN:HD22	1:C:456:ASN:H	1.45	0.64
1:C:527:GLY:HA3	1:C:562:ASN:HD21	1.63	0.64
1:D:562:ASN:ND2	1:D:562:ASN:H	1.96	0.64
1:F:186:ASN:HD21	1:F:204:TYR:H	1.46	0.64
1:F:368:LEU:HB2	1:F:424:MET:HE3	1.78	0.64
1:A:449:THR:HG21	1:B:407:GLY:N	2.13	0.64
1:C:540:SER:H	1:C:543:GLN:NE2	1.97	0.63
1:D:286:LYS:H	1:D:323:PRO:HG2	1.61	0.63
1:F:20:TYR:HB2	1:F:37:VAL:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ASP:OD2	1:C:333:ASN:HB2	1.98	0.63
1:A:344:VAL:HG21	1:A:394:VAL:HG21	1.79	0.63
1:C:61:ASN:HD21	1:C:548:THR:CG2	2.11	0.63
1:D:443:ARG:HB2	1:D:446:GLN:HG3	1.79	0.63
1:A:406:VAL:O	1:B:113:MET:HG3	1.99	0.63
1:B:50:ASN:H	1:B:50:ASN:ND2	1.92	0.63
1:E:344:VAL:HG21	1:E:394:VAL:HG21	1.81	0.63
1:F:61:ASN:ND2	1:F:548:THR:HG22	2.13	0.63
1:A:50:ASN:H	1:A:50:ASN:ND2	1.95	0.63
1:E:443:ARG:H	1:E:446:GLN:NE2	1.90	0.63
1:F:344:VAL:HG23	1:F:370:VAL:CG2	2.29	0.63
1:C:538:GLU:C	1:C:539:ILE:HG13	2.23	0.63
1:D:50:ASN:HD22	1:D:50:ASN:H	1.46	0.63
1:C:223:VAL:HG23	1:C:265:VAL:HG21	1.81	0.62
1:D:559:TYR:CZ	1:D:574:GLY:HA3	2.34	0.62
1:E:277:ASP:OD1	1:E:279:LYS:HG2	1.99	0.62
1:A:432:THR:HG21	1:A:436:PRO:HG3	1.80	0.62
1:D:366:GLN:HE22	1:D:424:MET:N	1.94	0.62
1:E:25:SER:HB3	1:E:81:PRO:HD3	1.81	0.62
1:E:559:TYR:CZ	1:E:574:GLY:HA3	2.34	0.62
1:D:371:GLN:N	1:D:415:GLN:HE22	1.80	0.62
1:F:94:TYR:CD1	1:F:107:ARG:HD3	2.35	0.62
1:C:145:ALA:HB3	1:C:165:THR:OG1	2.00	0.62
1:E:527:GLY:HA3	1:E:562:ASN:ND2	2.15	0.62
1:A:320:GLY:HA3	1:A:338:LEU:HD13	1.82	0.61
1:B:181:VAL:HG21	1:B:231:ILE:HD13	1.82	0.61
1:C:407:GLY:H	1:D:449:THR:HG21	1.65	0.61
1:D:540:SER:H	1:D:543:GLN:NE2	1.97	0.61
1:E:504:LYS:HG2	1:E:577:LEU:HB2	1.80	0.61
1:A:412:GLU:HG3	1:A:435:GLU:HA	1.82	0.61
1:D:20:TYR:HB2	1:D:37:VAL:HB	1.81	0.61
1:B:456:ASN:HD22	1:B:456:ASN:H	1.48	0.61
1:E:50:ASN:HD22	1:E:50:ASN:N	1.94	0.61
1:C:304:GLU:HB3	1:C:306:LYS:HG3	1.82	0.61
1:E:29:GLN:HB2	1:E:434:ALA:HB1	1.81	0.61
1:F:28:HIS:HA	1:F:77:ASP:HA	1.83	0.61
1:A:186:ASN:HD21	1:A:204:TYR:H	1.48	0.61
1:C:443:ARG:H	1:C:446:GLN:NE2	1.94	0.61
1:C:451:LYS:HE2	1:D:410:HIS:NE2	2.15	0.61
1:A:495:ALA:CB	1:A:496:PRO:CD	2.79	0.61
1:E:470:ASP:HB3	1:E:481:ILE:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:ASN:O	1:D:286:LYS:HE2	2.00	0.61
1:D:495:ALA:CB	1:D:496:PRO:CD	2.78	0.61
1:F:495:ALA:CB	1:F:496:PRO:CD	2.78	0.61
1:E:186:ASN:HD21	1:E:204:TYR:H	1.49	0.60
1:E:493:SER:O	1:E:494:VAL:HG13	2.01	0.60
1:E:492:THR:HG22	1:E:499:GLY:HA3	1.81	0.60
1:E:496:PRO:HD3	1:E:566:HIS:CD2	2.36	0.60
1:A:395:LEU:HD12	1:A:395:LEU:N	2.15	0.60
1:D:344:VAL:HG23	1:D:370:VAL:CG2	2.31	0.60
1:A:407:GLY:H	1:B:449:THR:HG21	1.66	0.60
1:A:79:HIS:H	1:A:98:ASN:HD21	1.49	0.60
1:C:202:THR:HG23	1:C:272:LEU:HB2	1.82	0.60
1:C:295:ALA:HB2	1:C:314:VAL:CG2	2.32	0.60
1:F:327:THR:HG22	1:F:377:ASN:ND2	2.16	0.60
1:F:372:TYR:O	1:F:396:SER:HB3	2.01	0.60
1:E:410:HIS:HE1	1:F:451:LYS:HE3	1.67	0.59
1:F:495:ALA:HB1	1:F:496:PRO:HD2	1.84	0.59
1:C:67:LEU:HD23	1:C:118:ILE:CD1	2.32	0.59
1:C:227:ASN:O	1:C:231:ILE:HG13	2.02	0.59
1:B:200:THR:HG22	1:B:225:VAL:HG22	1.85	0.59
1:C:295:ALA:HB2	1:C:314:VAL:HG21	1.84	0.59
1:D:61:ASN:HD21	1:D:548:THR:CG2	2.14	0.59
1:E:412:GLU:HG3	1:E:435:GLU:HA	1.84	0.59
1:B:323:PRO:HA	1:B:337:THR:O	2.02	0.59
1:F:181:VAL:HG21	1:F:231:ILE:HD13	1.84	0.59
1:A:200:THR:CG2	1:A:225:VAL:HG22	2.33	0.59
1:E:343:GLN:NE2	1:E:367:LYS:HD3	2.17	0.59
1:F:202:THR:HG23	1:F:272:LEU:HB2	1.84	0.59
1:B:527:GLY:HA3	1:B:562:ASN:ND2	2.17	0.59
1:C:470:ASP:HB3	1:C:481:ILE:HD13	1.84	0.59
1:B:202:THR:HG23	1:B:272:LEU:HB2	1.84	0.59
1:D:265:VAL:HG13	1:D:266:PRO:HD2	1.83	0.59
1:B:376:HIS:HB2	1:B:437:HIS:O	2.03	0.59
1:E:491:MET:HB2	1:E:515:ILE:HD13	1.85	0.59
1:B:512:THR:HG23	1:B:548:THR:HG22	1.84	0.59
1:F:47:PRO:HA	1:F:50:ASN:HD21	1.67	0.59
1:F:291:VAL:O	1:F:316:GLU:HA	2.03	0.59
1:A:109:ARG:HD2	1:A:111:ASP:OD1	2.03	0.58
1:C:61:ASN:HD21	1:C:548:THR:HG22	1.68	0.58
1:E:48:VAL:H	1:E:50:ASN:ND2	2.02	0.58
1:A:540:SER:H	1:A:543:GLN:HE21	1.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:THR:HB	1:D:374:PRO:HB2	1.83	0.58
1:A:468:GLU:HB2	6:A:2275:HOH:O	2.03	0.58
1:C:344:VAL:HG23	1:C:370:VAL:CG2	2.34	0.58
1:C:371:GLN:H	1:C:415:GLN:NE2	1.93	0.58
1:E:83:ILE:HB	6:E:2028:HOH:O	2.03	0.58
1:E:373:GLN:HE21	1:E:398:PHE:HD2	1.48	0.58
1:A:366:GLN:HE22	1:A:424:MET:N	1.99	0.58
1:B:79:HIS:H	1:B:98:ASN:ND2	2.01	0.58
1:E:478:ASN:HD21	1:E:492:THR:CG2	2.17	0.58
1:A:207:GLU:HG3	1:A:218:ASN:ND2	2.19	0.58
1:F:290:THR:HG22	1:F:318:GLU:HA	1.86	0.58
1:C:521:VAL:HB	1:C:524:VAL:HG21	1.84	0.58
1:C:534:GLY:HA2	1:D:75:ASN:HD21	1.68	0.58
1:C:75:ASN:HD22	1:C:75:ASN:H	1.51	0.58
1:C:342:SER:HA	1:C:374:PRO:HD3	1.84	0.58
1:C:525:THR:HG23	1:C:540:SER:HA	1.85	0.58
1:E:570:MET:HG3	6:F:2098:HOH:O	2.03	0.58
1:C:540:SER:H	1:C:543:GLN:HE21	1.51	0.57
1:F:494:VAL:HG12	1:F:518:LEU:HB2	1.86	0.57
1:C:472:VAL:HG12	1:C:479:LYS:HD2	1.86	0.57
1:E:323:PRO:HA	1:E:337:THR:O	2.03	0.57
1:A:25:SER:HB3	1:A:81:PRO:HD3	1.85	0.57
1:F:35:LEU:HD22	1:F:42:GLU:HA	1.85	0.57
1:A:371:GLN:HG2	1:A:402:ARG:NH1	2.19	0.57
1:C:395:LEU:HD22	1:C:437:HIS:O	2.04	0.57
1:F:302:LEU:HD22	1:F:312:THR:HG21	1.85	0.57
1:A:231:ILE:O	1:A:235:VAL:HG23	2.04	0.57
1:C:261:ARG:HG2	1:C:302:LEU:HG	1.85	0.57
1:F:282:ILE:HG23	1:F:291:VAL:HG13	1.86	0.57
1:D:562:ASN:H	1:D:562:ASN:HD22	1.52	0.57
1:E:498:TYR:CE1	1:E:572:MET:HG2	2.39	0.57
1:A:504:LYS:HG2	1:A:577:LEU:HB2	1.86	0.57
1:C:540:SER:HB3	1:C:541:PRO:HD2	1.85	0.57
1:D:186:ASN:H	1:D:186:ASN:HD22	1.51	0.57
1:A:453:TYR:CD2	1:A:543:GLN:HB2	2.39	0.57
1:D:25:SER:HB3	1:D:81:PRO:HD3	1.87	0.57
1:D:538:GLU:C	1:D:539:ILE:HG13	2.28	0.57
1:F:279:LYS:HB2	6:F:2096:HOH:O	2.03	0.57
1:C:80:HIS:H	1:C:98:ASN:ND2	2.03	0.57
1:C:410:HIS:HB2	1:D:523:ASP:OD1	2.05	0.57
1:E:339:PHE:CE1	1:E:373:GLN:HB3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:CG2	1:B:225:VAL:HG22	2.34	0.56
1:C:491:MET:HB2	1:C:515:ILE:HD13	1.88	0.56
1:E:478:ASN:HD21	1:E:492:THR:HG22	1.70	0.56
1:F:81:PRO:HB3	1:F:97:ILE:HD12	1.87	0.56
1:B:241:LYS:HG2	6:B:2146:HOH:O	2.05	0.56
1:F:75:ASN:H	1:F:75:ASN:HD22	1.52	0.56
1:A:80:HIS:H	1:A:98:ASN:HD21	1.51	0.56
1:B:200:THR:HG22	1:B:225:VAL:HA	1.86	0.56
1:B:343:GLN:NE2	1:B:367:LYS:HD3	2.20	0.56
1:B:456:ASN:H	1:B:456:ASN:ND2	2.02	0.56
1:C:302:LEU:HD22	1:C:312:THR:HG21	1.87	0.56
1:C:494:VAL:CG1	1:C:518:LEU:HB2	2.36	0.56
1:F:80:HIS:H	1:F:98:ASN:HD21	1.51	0.56
1:F:200:THR:HG22	1:F:225:VAL:HA	1.87	0.56
1:A:337:THR:HB	1:A:374:PRO:HB2	1.87	0.56
1:B:56:GLY:O	1:B:60:THR:HG23	2.06	0.56
1:B:372:TYR:O	1:B:396:SER:HB3	2.05	0.56
1:B:395:LEU:N	1:B:395:LEU:HD12	2.21	0.56
1:E:80:HIS:H	1:E:98:ASN:ND2	2.03	0.56
1:E:266:PRO:HG2	6:E:2129:HOH:O	2.04	0.56
1:A:485:ASN:HB2	6:A:2289:HOH:O	2.04	0.56
1:B:492:THR:HG22	1:B:499:GLY:HA3	1.87	0.56
1:C:494:VAL:HG12	1:C:518:LEU:HB2	1.87	0.56
1:D:304:GLU:HB3	1:D:306:LYS:HG3	1.87	0.56
1:D:342:SER:HA	1:D:374:PRO:HD3	1.87	0.56
1:A:200:THR:HG22	1:A:225:VAL:HG22	1.86	0.56
1:A:304:GLU:HB3	1:A:306:LYS:HG3	1.87	0.56
1:C:53:SER:OG	1:D:75:ASN:HB2	2.06	0.56
1:A:15:GLY:HA2	1:B:402:ARG:NH2	2.21	0.56
1:C:366:GLN:NE2	1:C:424:MET:H	2.01	0.56
1:F:432:THR:HG21	1:F:436:PRO:HG3	1.87	0.56
1:B:261:ARG:HG2	1:B:302:LEU:HG	1.88	0.56
1:D:85:MET:HE1	1:D:134:LYS:HG2	1.87	0.56
1:D:295:ALA:HB3	1:D:298:LYS:HD2	1.87	0.56
1:E:432:THR:HG21	1:E:436:PRO:HG3	1.86	0.55
1:E:472:VAL:HG12	1:E:479:LYS:HD2	1.88	0.55
1:E:523:ASP:OD1	1:F:410:HIS:HB2	2.07	0.55
1:B:456:ASN:HD22	1:B:456:ASN:N	2.04	0.55
1:E:449:THR:HG21	1:F:407:GLY:H	1.71	0.55
1:E:562:ASN:ND2	1:E:562:ASN:H	2.04	0.55
1:B:94:TYR:CD1	1:B:107:ARG:HD3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ASN:HD22	1:C:75:ASN:N	2.05	0.55
1:B:495:ALA:CB	1:B:496:PRO:CD	2.85	0.55
1:C:432:THR:HG21	1:C:436:PRO:HG3	1.88	0.55
1:F:559:TYR:CZ	1:F:574:GLY:HA3	2.42	0.55
1:A:61:ASN:HD21	1:A:548:THR:CG2	2.20	0.55
1:E:395:LEU:HD22	1:E:437:HIS:O	2.07	0.55
1:F:527:GLY:HA3	1:F:562:ASN:ND2	2.22	0.55
1:B:279:LYS:HB2	6:B:2156:HOH:O	2.07	0.55
1:A:559:TYR:CZ	1:A:574:GLY:HA3	2.42	0.55
1:B:337:THR:HB	1:B:374:PRO:HB2	1.89	0.55
1:C:18:ASP:HB3	1:C:37:VAL:O	2.06	0.55
1:A:181:VAL:HG21	1:A:231:ILE:HD13	1.89	0.54
1:A:494:VAL:CG1	1:A:518:LEU:HB2	2.38	0.54
1:D:79:HIS:H	1:D:98:ASN:ND2	2.06	0.54
1:A:512:THR:OG1	1:A:548:THR:HB	2.06	0.54
1:B:57:TRP:CH2	1:B:115:THR:HB	2.42	0.54
1:B:371:GLN:H	1:B:415:GLN:NE2	2.00	0.54
1:B:535:VAL:HG13	1:B:547:VAL:HG21	1.88	0.54
1:C:478:ASN:HD21	1:C:492:THR:HG22	1.71	0.54
1:D:288:SER:C	1:D:290:THR:H	2.15	0.54
1:D:266:PRO:HB2	1:D:288:SER:CB	2.38	0.54
1:A:344:VAL:HG23	1:A:370:VAL:CG2	2.33	0.54
1:F:392:LEU:HB2	1:F:419:ILE:HD13	1.88	0.54
1:A:186:ASN:ND2	1:A:205:ASN:H	2.05	0.54
1:A:267:LYS:HB3	1:A:287:LEU:HB2	1.87	0.54
1:A:395:LEU:HD22	1:A:437:HIS:O	2.08	0.54
1:C:470:ASP:HB3	1:C:481:ILE:CD1	2.37	0.54
1:D:37:VAL:HG21	1:D:441:LEU:HD22	1.89	0.54
1:F:61:ASN:ND2	6:F:2026:HOH:O	2.41	0.54
1:C:543:GLN:HG2	1:C:544:THR:N	2.21	0.54
1:D:188:ASP:HB3	1:D:202:THR:OG1	2.08	0.54
1:D:472:VAL:HG12	1:D:479:LYS:HD2	1.90	0.54
1:C:523:ASP:OD1	1:D:410:HIS:HB2	2.06	0.54
1:F:79:HIS:H	1:F:98:ASN:HD21	1.54	0.54
1:A:368:LEU:HB2	1:A:424:MET:HE3	1.89	0.54
1:B:562:ASN:ND2	1:B:562:ASN:H	2.06	0.54
1:D:372:TYR:O	1:D:396:SER:HB3	2.07	0.54
1:F:412:GLU:HG3	1:F:436:PRO:HD2	1.90	0.54
1:F:528:PHE:O	1:F:536:SER:HA	2.08	0.54
1:A:158:PHE:O	1:B:575:ARG:NH2	2.41	0.54
1:A:29:GLN:HB2	1:A:434:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:SER:HB3	1:C:81:PRO:HD3	1.90	0.53
1:D:302:LEU:HD22	1:D:312:THR:HG21	1.90	0.53
1:A:371:GLN:N	1:A:415:GLN:HE22	1.97	0.53
1:D:267:LYS:HB3	1:D:287:LEU:HB2	1.89	0.53
1:F:371:GLN:H	1:F:415:GLN:NE2	1.99	0.53
1:B:48:VAL:H	1:B:50:ASN:HD21	1.55	0.53
1:B:78:CYS:HB2	1:B:97:ILE:CD1	2.38	0.53
1:E:371:GLN:HG2	1:E:402:ARG:CZ	2.38	0.53
1:F:227:ASN:O	1:F:231:ILE:HG13	2.08	0.53
1:A:302:LEU:HD22	1:A:312:THR:HG21	1.90	0.53
1:C:395:LEU:H	1:C:395:LEU:HD12	1.73	0.53
1:E:20:TYR:HB2	1:E:37:VAL:HB	1.89	0.53
1:C:339:PHE:CE1	1:C:373:GLN:HB3	2.44	0.53
1:D:35:LEU:HD23	1:D:42:GLU:HA	1.91	0.53
1:B:304:GLU:HB3	1:B:306:LYS:HG3	1.88	0.53
1:B:415:GLN:HB3	1:B:426:LEU:HD11	1.89	0.53
1:B:494:VAL:CG1	1:B:518:LEU:HB2	2.39	0.53
1:C:263:ILE:O	1:C:265:VAL:HG23	2.09	0.53
1:F:144:ASN:HB3	1:F:187:LEU:HB3	1.91	0.53
1:A:478:ASN:HD21	1:A:492:THR:CG2	2.20	0.53
1:D:528:PHE:O	1:D:536:SER:HA	2.08	0.53
1:F:124:VAL:HG13	1:F:125:GLN:N	2.22	0.53
1:A:456:ASN:H	1:A:456:ASN:HD22	1.57	0.53
1:B:75:ASN:HD22	1:B:75:ASN:H	1.57	0.53
1:E:527:GLY:HA3	1:E:562:ASN:HD21	1.73	0.53
1:F:342:SER:HA	1:F:374:PRO:HD3	1.91	0.53
1:B:28:HIS:HA	1:B:77:ASP:HA	1.91	0.53
1:B:452:ILE:HD13	1:B:542:GLN:HG3	1.91	0.53
1:D:562:ASN:HD22	1:D:562:ASN:N	2.05	0.53
1:E:406:VAL:O	1:F:113:MET:HG3	2.09	0.53
1:E:467:ALA:HB1	1:E:472:VAL:HG23	1.91	0.53
1:C:495:ALA:CB	1:C:496:PRO:HD2	2.37	0.53
1:B:29:GLN:HB2	1:B:434:ALA:HB3	1.91	0.52
1:D:29:GLN:HB2	1:D:434:ALA:HB3	1.90	0.52
1:D:50:ASN:H	1:D:50:ASN:ND2	2.07	0.52
1:D:286:LYS:N	1:D:323:PRO:HG2	2.24	0.52
1:E:48:VAL:H	1:E:50:ASN:HD21	1.57	0.52
1:F:528:PHE:CD2	1:F:537:MET:HE2	2.44	0.52
1:C:534:GLY:HA2	1:D:75:ASN:ND2	2.24	0.52
1:D:343:GLN:HA	1:D:370:VAL:HG23	1.90	0.52
1:D:517:ASN:HB2	1:D:539:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:PHE:HA	1:D:374:PRO:HD2	1.92	0.52
1:F:79:HIS:H	1:F:98:ASN:ND2	2.07	0.52
1:F:456:ASN:C	1:F:456:ASN:HD22	2.16	0.52
1:B:538:GLU:C	1:B:539:ILE:HG13	2.33	0.52
1:C:296:ILE:HG23	1:C:299:LEU:HD12	1.92	0.52
1:A:75:ASN:H	1:A:75:ASN:HD22	1.55	0.52
1:B:302:LEU:HD22	1:B:312:THR:HG21	1.91	0.52
1:B:343:GLN:HE22	1:B:367:LYS:HD3	1.75	0.52
1:D:202:THR:HG23	1:D:272:LEU:HB2	1.92	0.52
1:D:494:VAL:HG13	1:D:518:LEU:HB2	1.92	0.52
1:C:130:LEU:HD23	1:C:130:LEU:C	2.35	0.52
1:D:494:VAL:CG1	1:D:518:LEU:HB2	2.39	0.52
1:E:534:GLY:HA2	1:F:75:ASN:ND2	2.23	0.52
1:F:454:GLU:HB3	6:F:2156:HOH:O	2.10	0.52
1:A:412:GLU:HG3	1:A:436:PRO:HD2	1.92	0.52
1:B:371:GLN:HG2	1:B:402:ARG:HD2	1.92	0.52
1:D:117:LYS:HB2	1:D:175:MET:HG3	1.91	0.52
1:D:495:ALA:CB	1:D:496:PRO:HD2	2.37	0.52
1:E:231:ILE:O	1:E:235:VAL:HG23	2.09	0.52
1:A:443:ARG:H	1:A:446:GLN:NE2	2.02	0.52
1:D:18:ASP:HB3	1:D:37:VAL:O	2.09	0.52
1:E:344:VAL:HG23	1:E:370:VAL:CG2	2.38	0.52
1:E:372:TYR:O	1:E:396:SER:HB3	2.10	0.52
1:C:93:LYS:HE2	1:C:94:TYR:CZ	2.44	0.51
1:F:83:ILE:HG22	1:F:440:ILE:HD13	1.91	0.51
1:A:202:THR:HG23	1:A:272:LEU:HB2	1.93	0.51
1:C:372:TYR:O	1:C:396:SER:HB3	2.11	0.51
1:E:158:PHE:O	1:F:575:ARG:NH2	2.43	0.51
1:E:295:ALA:HB2	1:E:314:VAL:HG21	1.92	0.51
1:A:443:ARG:N	1:A:446:GLN:HE21	2.02	0.51
1:B:373:GLN:HE21	1:B:398:PHE:HD2	1.57	0.51
1:B:390:LYS:HG2	6:B:2010:HOH:O	2.09	0.51
1:C:495:ALA:CB	1:C:496:PRO:CD	2.86	0.51
1:E:517:ASN:HB2	1:E:539:ILE:HG22	1.91	0.51
1:F:261:ARG:CZ	1:F:303:PHE:HA	2.40	0.51
1:C:50:ASN:H	1:C:50:ASN:ND2	2.06	0.51
1:E:528:PHE:O	1:E:536:SER:HA	2.10	0.51
1:B:186:ASN:HD21	1:B:204:TYR:H	1.59	0.51
1:A:495:ALA:CB	1:A:496:PRO:HD2	2.39	0.51
1:D:80:HIS:H	1:D:98:ASN:ND2	2.08	0.51
1:D:186:ASN:HD22	1:D:186:ASN:N	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:ASN:ND2	1:D:205:ASN:H	2.09	0.51
1:E:407:GLY:H	1:F:449:THR:HG21	1.76	0.51
1:F:295:ALA:HB2	1:F:314:VAL:HG21	1.93	0.51
1:A:291:VAL:O	1:A:316:GLU:HA	2.11	0.51
1:C:288:SER:C	1:C:290:THR:H	2.18	0.51
1:E:18:ASP:HB3	1:E:37:VAL:O	2.11	0.51
1:E:325:HIS:CE1	1:E:376:HIS:CE1	2.99	0.51
1:E:566:HIS:HB2	6:E:2222:HOH:O	2.11	0.51
1:A:339:PHE:CE1	1:A:373:GLN:HB3	2.46	0.51
1:A:535:VAL:HG13	1:A:547:VAL:HG21	1.92	0.51
1:B:432:THR:HG21	1:B:436:PRO:HG3	1.92	0.51
1:C:78:CYS:HA	1:C:98:ASN:O	2.11	0.51
1:C:125:GLN:HE22	1:D:558:TRP:H	1.57	0.51
1:C:231:ILE:O	1:C:235:VAL:HG23	2.10	0.51
1:F:29:GLN:HB2	1:F:434:ALA:CB	2.40	0.51
1:F:152:PRO:HG2	1:F:154:ASP:OD2	2.11	0.51
1:D:279:LYS:HB2	6:D:2054:HOH:O	2.10	0.51
1:A:261:ARG:HG2	1:A:302:LEU:HG	1.92	0.50
1:C:78:CYS:HB2	1:C:97:ILE:CD1	2.41	0.50
1:D:90:TYR:CD2	1:D:442:VAL:HG12	2.46	0.50
1:D:109:ARG:NH2	1:D:112:ILE:HD13	2.26	0.50
1:E:53:SER:OG	1:F:75:ASN:HB2	2.11	0.50
1:E:78:CYS:HB2	1:E:97:ILE:CD1	2.42	0.50
1:A:495:ALA:HB3	6:A:2294:HOH:O	2.11	0.50
1:B:29:GLN:HB2	1:B:434:ALA:HB1	1.93	0.50
1:B:80:HIS:H	1:B:98:ASN:HD21	1.60	0.50
1:C:37:VAL:HG21	1:C:441:LEU:HD22	1.92	0.50
1:C:478:ASN:HD21	1:C:492:THR:CG2	2.23	0.50
1:A:288:SER:C	1:A:290:THR:H	2.19	0.50
1:C:404:LEU:HD11	1:D:18:ASP:HB2	1.93	0.50
1:F:96:PHE:CE2	1:F:107:ARG:HG3	2.46	0.50
1:A:564:PHE:HB2	1:B:435:GLU:OE2	2.12	0.50
1:B:25:SER:HB3	1:B:81:PRO:HD3	1.93	0.50
1:C:78:CYS:HB2	1:C:97:ILE:HG12	1.93	0.50
1:E:75:ASN:HD22	1:E:75:ASN:H	1.58	0.50
1:E:109:ARG:HH21	1:E:112:ILE:CD1	2.24	0.50
1:E:109:ARG:HH21	1:E:112:ILE:HD13	1.76	0.50
1:F:186:ASN:ND2	1:F:205:ASN:H	2.10	0.50
1:F:470:ASP:HB3	1:F:481:ILE:CD1	2.41	0.50
1:A:57:TRP:CH2	1:A:115:THR:HB	2.46	0.50
1:A:485:ASN:HB3	6:A:2302:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:GLY:HA3	1:A:562:ASN:ND2	2.27	0.50
1:E:21:TYR:HB2	1:E:442:VAL:CG2	2.42	0.50
1:F:50:ASN:H	1:F:50:ASN:ND2	2.03	0.50
1:F:57:TRP:CH2	1:F:115:THR:HB	2.47	0.50
1:F:277:ASP:OD1	1:F:279:LYS:HG2	2.10	0.50
1:F:344:VAL:HG21	1:F:394:VAL:HG21	1.94	0.50
1:A:45:ARG:NH2	6:A:2013:HOH:O	2.25	0.50
1:B:125:GLN:HG3	1:B:149:ILE:HD13	1.93	0.50
1:E:260:THR:O	1:E:261:ARG:HD2	2.12	0.50
1:A:37:VAL:HG21	1:A:441:LEU:HD22	1.94	0.50
1:D:186:ASN:HD21	1:D:205:ASN:H	1.59	0.50
1:E:548:THR:HG21	6:E:2012:HOH:O	2.10	0.50
1:F:261:ARG:HG2	1:F:302:LEU:HG	1.94	0.50
1:F:343:GLN:HE21	1:F:367:LYS:HD3	1.75	0.50
1:F:371:GLN:N	1:F:415:GLN:HE22	1.99	0.50
1:F:530:MET:SD	1:F:559:TYR:HB3	2.52	0.50
1:A:279:LYS:HB2	6:A:2178:HOH:O	2.11	0.50
1:B:339:PHE:CE1	1:B:373:GLN:HB3	2.47	0.50
1:C:200:THR:CG2	1:C:225:VAL:HG22	2.42	0.50
1:D:165:THR:HG21	1:D:186:ASN:HA	1.93	0.50
1:A:449:THR:HB	6:A:2262:HOH:O	2.12	0.49
1:D:553:LYS:HG3	6:D:2110:HOH:O	2.12	0.49
1:E:107:ARG:NH1	1:E:116:ASP:OD2	2.43	0.49
1:E:543:GLN:HG2	1:E:544:THR:N	2.27	0.49
1:C:339:PHE:HA	1:C:374:PRO:HD2	1.94	0.49
1:D:29:GLN:HB2	1:D:434:ALA:CB	2.41	0.49
1:D:343:GLN:NE2	1:D:367:LYS:HD3	2.27	0.49
1:D:376:HIS:HB2	1:D:437:HIS:O	2.11	0.49
1:A:343:GLN:NE2	1:A:367:LYS:HD3	2.27	0.49
1:F:75:ASN:HD22	1:F:75:ASN:N	2.09	0.49
1:F:281:PHE:CD2	1:F:296:ILE:HG12	2.47	0.49
1:C:322:GLY:N	1:C:323:PRO:HD3	2.27	0.49
1:A:227:ASN:O	1:A:231:ILE:HG13	2.12	0.49
1:A:212:LEU:HD12	1:B:497:GLN:OE1	2.13	0.49
1:B:202:THR:HG23	1:B:272:LEU:HD12	1.94	0.49
1:B:282:ILE:HG23	1:B:291:VAL:HG13	1.93	0.49
1:B:495:ALA:O	6:B:2265:HOH:O	2.19	0.49
1:C:35:LEU:HD23	1:C:42:GLU:HA	1.94	0.49
1:F:540:SER:HB3	1:F:541:PRO:HD2	1.95	0.49
1:C:29:GLN:HB2	1:C:434:ALA:HB3	1.93	0.49
1:D:21:TYR:HB2	1:D:442:VAL:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ARG:HD2	1:D:191:ASP:CG	2.38	0.49
1:E:80:HIS:H	1:E:98:ASN:HD21	1.59	0.49
1:F:35:LEU:CD2	1:F:42:GLU:HA	2.43	0.49
1:F:495:ALA:C	6:F:2182:HOH:O	2.55	0.49
1:A:537:MET:HE2	1:A:547:VAL:HG12	1.94	0.49
1:B:210:VAL:HG12	6:B:2133:HOH:O	2.13	0.49
1:B:540:SER:HB3	1:B:541:PRO:CD	2.43	0.49
1:C:343:GLN:NE2	1:C:367:LYS:HD3	2.27	0.49
1:C:528:PHE:O	1:C:536:SER:HA	2.13	0.49
1:E:94:TYR:CD1	1:E:107:ARG:HD3	2.47	0.49
1:A:371:GLN:HG2	1:A:402:ARG:HD2	1.96	0.48
1:C:197:LYS:HG3	1:C:229:GLU:HB2	1.95	0.48
1:E:494:VAL:CG1	1:E:518:LEU:HB2	2.43	0.48
1:F:50:ASN:HD22	1:F:50:ASN:N	2.02	0.48
1:A:411:PRO:HB3	1:B:43:LEU:O	2.13	0.48
1:E:217:ARG:HD2	6:E:2095:HOH:O	2.13	0.48
1:F:495:ALA:CB	1:F:496:PRO:HD2	2.43	0.48
1:A:197:LYS:HG3	1:A:229:GLU:HB2	1.95	0.48
1:B:75:ASN:HD22	1:B:75:ASN:N	2.10	0.48
1:B:575:ARG:HD3	6:B:2274:HOH:O	2.12	0.48
1:D:191:ASP:OD1	1:D:192:ALA:N	2.45	0.48
1:D:261:ARG:HG2	1:D:302:LEU:HG	1.95	0.48
1:E:125:GLN:HE22	1:F:558:TRP:H	1.61	0.48
1:E:200:THR:CG2	1:E:225:VAL:HG22	2.43	0.48
1:F:343:GLN:HB3	1:F:369:ASP:HA	1.94	0.48
1:B:223:VAL:HG23	1:B:265:VAL:HG21	1.95	0.48
1:C:35:LEU:CD2	1:C:42:GLU:HA	2.43	0.48
1:D:85:MET:CE	1:D:134:LYS:HG2	2.43	0.48
1:D:543:GLN:HG2	1:D:544:THR:N	2.29	0.48
1:B:371:GLN:HG2	1:B:402:ARG:NH1	2.29	0.48
1:C:21:TYR:HB2	1:C:442:VAL:CG2	2.44	0.48
1:C:449:THR:HG21	1:D:407:GLY:H	1.77	0.48
1:D:296:ILE:HG23	1:D:299:LEU:HD12	1.95	0.48
1:A:130:LEU:C	1:A:130:LEU:HD23	2.39	0.48
1:A:407:GLY:N	1:B:449:THR:HG21	2.28	0.48
1:A:538:GLU:HB2	1:A:563:TRP:CH2	2.48	0.48
1:B:47:PRO:HA	1:B:50:ASN:HD21	1.78	0.48
1:B:559:TYR:CZ	1:B:574:GLY:HA3	2.49	0.48
1:E:46:ILE:HG21	1:E:108:ILE:HD13	1.94	0.48
1:E:61:ASN:HD21	1:E:548:THR:CG2	2.26	0.48
1:E:78:CYS:HA	1:E:98:ASN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:VAL:HG13	1:E:136:PRO:HA	1.94	0.48
1:E:491:MET:HB2	1:E:515:ILE:CD1	2.43	0.48
1:F:135:VAL:HG13	1:F:136:PRO:HA	1.94	0.48
1:C:47:PRO:HA	1:C:50:ASN:HD21	1.77	0.48
1:D:295:ALA:HB2	1:D:314:VAL:HG21	1.94	0.48
1:E:109:ARG:HG3	1:E:116:ASP:HB2	1.95	0.48
1:A:301:ASP:OD1	1:A:306:LYS:HD2	2.12	0.48
1:B:98:ASN:H	1:B:98:ASN:HD22	1.60	0.48
1:B:467:ALA:HB1	1:B:472:VAL:HG22	1.96	0.48
1:E:109:ARG:NH2	1:E:112:ILE:HD13	2.29	0.48
1:E:371:GLN:H	1:E:415:GLN:NE2	1.94	0.48
1:B:491:MET:HB2	1:B:515:ILE:HD13	1.96	0.48
1:C:449:THR:HG22	1:C:450:LYS:N	2.29	0.48
1:E:83:ILE:HG22	1:E:440:ILE:HD13	1.95	0.48
1:F:329:ASP:OD2	1:F:333:ASN:HB2	2.14	0.48
1:A:370:VAL:HG13	1:A:415:GLN:NE2	2.29	0.48
1:D:78:CYS:HA	1:D:98:ASN:O	2.14	0.48
1:A:323:PRO:HA	1:A:337:THR:O	2.14	0.47
1:B:449:THR:HG21	6:B:2230:HOH:O	2.14	0.47
1:C:359:ASP:C	1:C:360:ARG:HG3	2.39	0.47
1:D:133:GLN:OE1	1:D:139:ASN:HB2	2.14	0.47
1:D:366:GLN:HE22	1:D:423:GLU:HA	1.79	0.47
1:F:18:ASP:HB3	1:F:37:VAL:O	2.14	0.47
1:F:282:ILE:HG23	1:F:291:VAL:CG1	2.42	0.47
1:C:540:SER:HB3	1:C:541:PRO:CD	2.44	0.47
1:C:291:VAL:O	1:C:316:GLU:HA	2.15	0.47
1:D:75:ASN:H	1:D:75:ASN:HD22	1.61	0.47
1:D:321:LEU:HD12	1:D:341:ASP:OD1	2.14	0.47
1:D:528:PHE:CD2	1:D:537:MET:HE2	2.49	0.47
1:A:29:GLN:HB2	1:A:434:ALA:CB	2.43	0.47
1:A:78:CYS:HA	1:A:98:ASN:O	2.14	0.47
1:A:202:THR:HG23	1:A:272:LEU:HD12	1.95	0.47
1:C:456:ASN:HD22	1:C:456:ASN:N	2.08	0.47
1:E:220:ARG:HD2	6:E:2100:HOH:O	2.13	0.47
1:E:443:ARG:N	1:E:446:GLN:HE21	1.92	0.47
1:F:202:THR:HG23	1:F:272:LEU:HD12	1.95	0.47
1:F:538:GLU:C	1:F:539:ILE:HG13	2.40	0.47
1:A:286:LYS:NZ	6:A:2179:HOH:O	2.47	0.47
1:C:80:HIS:H	1:C:98:ASN:HD21	1.62	0.47
1:C:284:ASN:ND2	1:C:325:HIS:HA	2.30	0.47
1:C:547:VAL:O	1:C:547:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:HIS:NE2	1:D:131:ARG:HG2	2.30	0.47
1:D:366:GLN:HG2	1:D:367:LYS:N	2.30	0.47
1:F:72:GLN:HG3	6:F:2035:HOH:O	2.13	0.47
1:A:287:LEU:HD21	1:B:568:LEU:HD21	1.97	0.47
1:B:186:ASN:HD22	1:B:186:ASN:H	1.62	0.47
1:C:212:LEU:HD11	1:D:496:PRO:HG2	1.96	0.47
1:C:304:GLU:HG2	1:C:306:LYS:HE2	1.97	0.47
1:F:449:THR:CG2	1:F:450:LYS:N	2.78	0.47
1:A:174:THR:HG21	6:A:2109:HOH:O	2.14	0.47
1:B:193:ASP:HB2	6:B:2125:HOH:O	2.13	0.47
1:B:302:LEU:HD11	1:B:309:LEU:HD23	1.96	0.47
1:D:29:GLN:HG3	1:D:33:ARG:HH21	1.79	0.47
1:D:207:GLU:HG3	1:D:218:ASN:ND2	2.30	0.47
1:E:295:ALA:HB2	1:E:314:VAL:CG2	2.43	0.47
1:E:403:PHE:HB3	1:F:43:LEU:HD22	1.97	0.47
1:E:494:VAL:HA	6:E:2213:HOH:O	2.15	0.47
1:F:11:HIS:HB3	6:F:2003:HOH:O	2.15	0.47
1:B:527:GLY:HA3	1:B:562:ASN:HD21	1.78	0.47
1:E:530:MET:SD	1:E:559:TYR:HB3	2.55	0.47
1:B:467:ALA:HB1	1:B:472:VAL:CG2	2.45	0.47
1:D:327:THR:HG22	1:D:335:TYR:HB2	1.97	0.47
1:D:344:VAL:HG21	1:D:394:VAL:HG21	1.96	0.47
1:F:144:ASN:HB3	1:F:187:LEU:CB	2.45	0.47
1:D:186:ASN:HD21	1:D:204:TYR:H	1.63	0.47
1:C:515:ILE:HG21	1:C:539:ILE:HD13	1.96	0.46
1:F:265:VAL:HG13	1:F:292:SER:OG	2.16	0.46
1:F:494:VAL:CG1	1:F:518:LEU:HB2	2.44	0.46
1:A:339:PHE:HA	1:A:374:PRO:HD2	1.97	0.46
1:C:397:LYS:HE2	6:C:2055:HOH:O	2.15	0.46
1:D:57:TRP:CH2	1:D:115:THR:HB	2.50	0.46
1:D:231:ILE:O	1:D:235:VAL:HG23	2.15	0.46
1:D:327:THR:HG22	1:D:377:ASN:ND2	2.30	0.46
1:D:456:ASN:H	1:D:456:ASN:HD22	1.62	0.46
1:A:75:ASN:HD22	1:A:75:ASN:N	2.12	0.46
1:B:470:ASP:CB	1:B:481:ILE:HD13	2.40	0.46
1:B:540:SER:H	1:B:543:GLN:NE2	2.13	0.46
1:D:450:LYS:HD3	6:D:2069:HOH:O	2.15	0.46
1:D:452:ILE:O	1:D:452:ILE:HG13	2.15	0.46
1:D:559:TYR:CE1	1:D:574:GLY:HA3	2.50	0.46
1:A:541:PRO:O	1:A:542:GLN:HB2	2.15	0.46
1:B:288:SER:C	1:B:290:THR:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:GLU:HG2	1:B:539:ILE:N	2.31	0.46
1:C:411:PRO:HB3	1:D:43:LEU:O	2.15	0.46
1:E:304:GLU:HB3	1:E:306:LYS:HG3	1.97	0.46
1:A:95:LEU:HD23	1:A:96:PHE:N	2.30	0.46
1:B:231:ILE:O	1:B:235:VAL:HG23	2.15	0.46
1:E:186:ASN:ND2	1:E:205:ASN:H	2.14	0.46
1:F:223:VAL:HG23	1:F:265:VAL:HG21	1.98	0.46
1:B:366:GLN:HG2	1:B:367:LYS:N	2.31	0.46
1:B:515:ILE:HG21	1:B:539:ILE:HD13	1.97	0.46
1:C:85:MET:HE1	1:C:134:LYS:HG2	1.98	0.46
1:C:117:LYS:HB2	1:C:175:MET:HG3	1.98	0.46
1:D:78:CYS:HB2	1:D:97:ILE:HG12	1.98	0.46
1:D:469:LYS:HD3	6:D:2081:HOH:O	2.15	0.46
1:F:143:CYS:SG	1:F:168:THR:HB	2.56	0.46
1:A:329:ASP:OD2	1:A:333:ASN:HB2	2.16	0.46
1:A:521:VAL:HG23	6:A:2307:HOH:O	2.16	0.46
1:B:37:VAL:HG13	1:B:38:PRO:HA	1.97	0.46
1:D:37:VAL:HG13	1:D:38:PRO:HA	1.98	0.46
1:A:61:ASN:HD21	1:A:548:THR:HG23	1.80	0.46
1:C:67:LEU:HD23	1:C:118:ILE:HD13	1.97	0.46
1:C:337:THR:HB	1:C:374:PRO:HB2	1.98	0.46
1:A:245:ASP:HB3	1:F:156:THR:HB	1.98	0.46
1:C:562:ASN:ND2	1:C:562:ASN:H	2.14	0.46
1:D:95:LEU:C	1:D:95:LEU:HD23	2.41	0.46
1:F:284:ASN:ND2	1:F:325:HIS:HA	2.31	0.46
1:A:376:HIS:HB2	1:A:437:HIS:O	2.15	0.45
1:B:296:ILE:HG23	1:B:299:LEU:HD12	1.98	0.45
1:B:338:LEU:HD12	1:B:343:GLN:HE21	1.80	0.45
1:B:386:ASP:O	1:B:387:ALA:C	2.59	0.45
1:C:407:GLY:H	1:D:449:THR:CG2	2.29	0.45
1:E:131:ARG:HD2	1:E:191:ASP:CG	2.41	0.45
1:E:464:ARG:HD3	6:E:2198:HOH:O	2.16	0.45
1:F:49:PHE:CZ	1:F:99:ASP:HB2	2.51	0.45
1:F:366:GLN:NE2	1:F:424:MET:H	2.11	0.45
1:F:372:TYR:CD1	1:F:400:LYS:HD2	2.50	0.45
1:C:142:PHE:HB3	1:C:167:PHE:CZ	2.51	0.45
1:C:266:PRO:HB2	6:C:2050:HOH:O	2.15	0.45
1:C:376:HIS:CE1	1:C:438:ASP:HB2	2.51	0.45
1:D:360:ARG:HE	1:D:360:ARG:HB2	1.51	0.45
1:E:181:VAL:HG21	1:E:231:ILE:HD13	1.97	0.45
1:B:535:VAL:CG1	1:B:547:VAL:HG11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:LYS:HG2	6:C:2003:HOH:O	2.15	0.45
1:D:547:VAL:O	1:D:547:VAL:HG13	2.15	0.45
1:F:117:LYS:HB2	1:F:175:MET:HG3	1.96	0.45
1:F:495:ALA:HA	6:F:2182:HOH:O	2.16	0.45
1:F:535:VAL:HG13	1:F:547:VAL:HG21	1.97	0.45
1:F:540:SER:HB3	1:F:541:PRO:CD	2.46	0.45
1:A:342:SER:HA	1:A:374:PRO:HD3	1.97	0.45
1:B:540:SER:HB3	1:B:541:PRO:HD2	1.99	0.45
1:C:75:ASN:ND2	1:D:534:GLY:HA2	2.22	0.45
1:D:28:HIS:HA	1:D:77:ASP:HA	1.98	0.45
1:D:291:VAL:O	1:D:316:GLU:HA	2.16	0.45
1:A:79:HIS:H	1:A:98:ASN:ND2	2.13	0.45
1:A:530:MET:SD	1:A:559:TYR:HB3	2.56	0.45
1:B:265:VAL:HG13	1:B:266:PRO:HD2	1.98	0.45
1:D:130:LEU:C	1:D:130:LEU:HD23	2.42	0.45
1:D:361:VAL:HG12	1:D:362:ASN:N	2.32	0.45
1:E:29:GLN:HB2	1:E:434:ALA:HB3	1.98	0.45
1:E:547:VAL:O	1:E:547:VAL:HG13	2.17	0.45
1:B:328:PHE:CD1	1:B:328:PHE:N	2.85	0.45
1:C:131:ARG:HD2	1:C:191:ASP:CG	2.42	0.45
1:C:221:ASP:O	1:C:264:PRO:HA	2.17	0.45
1:D:61:ASN:OD1	1:D:548:THR:HG22	2.16	0.45
1:D:575:ARG:HD3	6:D:2095:HOH:O	2.16	0.45
1:E:286:LYS:HD3	6:E:2125:HOH:O	2.17	0.45
1:F:221:ASP:O	1:F:264:PRO:HA	2.17	0.45
1:F:456:ASN:ND2	6:F:2156:HOH:O	2.49	0.45
1:A:188:ASP:HB3	1:A:202:THR:OG1	2.16	0.45
1:C:189:ASN:O	1:C:201:SER:HA	2.17	0.45
1:D:343:GLN:HB3	1:D:369:ASP:HA	1.99	0.45
1:E:562:ASN:H	1:E:562:ASN:HD22	1.65	0.45
1:F:29:GLN:HB2	1:F:434:ALA:HB3	1.99	0.45
1:F:288:SER:C	1:F:290:THR:H	2.24	0.45
1:B:349:ILE:HB	6:B:2178:HOH:O	2.17	0.45
1:E:105:VAL:HG21	1:E:143:CYS:SG	2.57	0.45
1:E:179:TRP:CZ3	1:E:231:ILE:HG21	2.52	0.45
1:E:321:LEU:HB3	1:E:340:ILE:HB	1.98	0.45
1:F:449:THR:HG22	1:F:450:LYS:N	2.32	0.45
1:F:538:GLU:HB2	1:F:563:TRP:CH2	2.51	0.45
1:A:133:GLN:OE1	1:A:139:ASN:HB2	2.17	0.45
1:A:373:GLN:HE21	1:A:398:PHE:HD2	1.65	0.45
1:A:562:ASN:C	1:A:562:ASN:HD22	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:ASN:H	1:B:562:ASN:HD22	1.64	0.45
1:C:151:GLN:HA	1:C:152:PRO:HA	1.85	0.45
1:C:165:THR:HG21	1:C:186:ASN:HA	1.99	0.45
1:C:210:VAL:HG12	6:C:2038:HOH:O	2.17	0.45
1:C:319:LEU:HD22	1:C:345:CYS:SG	2.56	0.45
1:F:83:ILE:CD1	1:F:92:GLY:HA2	2.28	0.45
1:F:142:PHE:HB3	1:F:167:PHE:CZ	2.52	0.45
1:A:371:GLN:HG2	1:A:402:ARG:CZ	2.46	0.45
1:B:286:LYS:H	1:B:323:PRO:HG2	1.82	0.45
1:C:193:ASP:OD2	1:C:198:TYR:HB2	2.17	0.45
1:C:262:TYR:O	1:C:264:PRO:HD3	2.17	0.45
1:E:200:THR:HG22	1:E:225:VAL:HG22	1.98	0.45
1:E:456:ASN:HD22	1:E:456:ASN:N	2.05	0.45
1:F:342:SER:HA	1:F:374:PRO:CD	2.47	0.45
1:F:495:ALA:HB3	6:F:2184:HOH:O	2.16	0.45
1:A:135:VAL:HG13	1:A:136:PRO:HA	1.99	0.44
1:A:523:ASP:OD1	1:B:410:HIS:HB2	2.17	0.44
1:C:268:ASN:O	1:C:286:LYS:HE2	2.17	0.44
1:D:521:VAL:HB	1:D:524:VAL:HG21	1.98	0.44
1:E:47:PRO:HA	1:E:50:ASN:HD21	1.82	0.44
1:E:133:GLN:OE1	1:E:139:ASN:HB2	2.16	0.44
1:E:202:THR:HG23	1:E:272:LEU:HD12	1.98	0.44
1:A:304:GLU:HG2	1:A:306:LYS:HE2	1.99	0.44
1:A:477:ASP:CG	1:A:479:LYS:HE3	2.42	0.44
1:C:381:LEU:HB2	1:C:387:ALA:HA	2.00	0.44
1:E:505:VAL:O	1:E:578:VAL:HA	2.16	0.44
1:F:495:ALA:HB1	1:F:496:PRO:HD3	1.96	0.44
1:F:540:SER:H	1:F:543:GLN:HE21	1.62	0.44
1:A:433:TYR:CG	1:A:434:ALA:N	2.86	0.44
1:A:456:ASN:HD22	1:A:456:ASN:N	2.14	0.44
1:A:494:VAL:O	1:A:495:ALA:C	2.59	0.44
1:B:134:LYS:HE3	6:B:2088:HOH:O	2.16	0.44
1:B:432:THR:HG22	1:B:433:TYR:N	2.33	0.44
1:B:433:TYR:CG	1:B:434:ALA:N	2.85	0.44
1:C:343:GLN:HA	1:C:370:VAL:H	1.82	0.44
1:E:286:LYS:NZ	6:E:2125:HOH:O	2.51	0.44
1:F:262:TYR:O	1:F:264:PRO:HD3	2.17	0.44
1:A:247:LYS:HE3	6:F:2063:HOH:O	2.17	0.44
1:B:495:ALA:CA	6:B:2265:HOH:O	2.65	0.44
1:D:223:VAL:HG23	1:D:265:VAL:HG21	1.99	0.44
1:F:302:LEU:HD11	1:F:309:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:PRO:HA	1:F:337:THR:O	2.17	0.44
1:A:435:GLU:OE2	1:B:564:PHE:HB2	2.17	0.44
1:B:370:VAL:HG13	1:B:415:GLN:NE2	2.31	0.44
1:B:494:VAL:O	1:B:495:ALA:C	2.60	0.44
1:C:61:ASN:ND2	1:C:548:THR:HG22	2.30	0.44
1:C:128:HIS:CE1	1:D:570:MET:HE1	2.53	0.44
1:E:320:GLY:HA3	1:E:338:LEU:HD13	1.98	0.44
1:F:95:LEU:C	1:F:95:LEU:HD23	2.43	0.44
1:B:495:ALA:CB	1:B:496:PRO:HD2	2.47	0.44
1:B:511:VAL:O	1:B:548:THR:HA	2.18	0.44
1:C:276:PRO:HD3	1:C:328:PHE:CG	2.53	0.44
1:E:531:VAL:HG11	1:F:125:GLN:HG2	1.99	0.44
1:A:95:LEU:HB2	1:A:110:LEU:HD21	2.00	0.44
1:A:160:LEU:HD11	1:A:210:VAL:HG12	1.99	0.44
1:B:370:VAL:HG13	6:B:2212:HOH:O	2.18	0.44
1:B:371:GLN:CB	1:B:402:ARG:HD2	2.48	0.44
1:C:28:HIS:HA	1:C:77:ASP:HA	1.99	0.44
1:C:29:GLN:HB2	1:C:434:ALA:CB	2.48	0.44
1:C:457:ASP:HA	1:C:458:PRO:HD3	1.88	0.44
1:D:39:SER:O	1:D:40:MET:HB2	2.16	0.44
1:E:553:LYS:HB2	1:E:554:PRO:HD2	2.00	0.44
1:A:147:PHE:HB3	1:B:558:TRP:CE2	2.52	0.44
1:B:395:LEU:HD12	1:B:395:LEU:H	1.83	0.44
1:C:491:MET:HB2	1:C:515:ILE:CD1	2.46	0.44
1:E:107:ARG:HB2	1:E:175:MET:HE2	2.00	0.44
1:E:202:THR:HG23	1:E:272:LEU:HB2	2.00	0.44
1:E:276:PRO:HD3	1:E:328:PHE:CG	2.53	0.44
1:A:75:ASN:ND2	1:A:102:ASN:HD21	2.16	0.43
1:A:433:TYR:CE2	1:A:434:ALA:HB2	2.53	0.43
1:B:95:LEU:C	1:B:95:LEU:HD23	2.43	0.43
1:B:207:GLU:HG3	1:B:218:ASN:ND2	2.33	0.43
1:F:529:CYS:O	1:F:559:TYR:HA	2.17	0.43
1:B:212:LEU:HD22	1:B:216:MET:SD	2.58	0.43
1:B:360:ARG:HE	1:B:360:ARG:HB2	1.69	0.43
1:B:540:SER:H	1:B:543:GLN:HE21	1.66	0.43
1:C:49:PHE:CE2	1:C:99:ASP:HB2	2.53	0.43
1:C:395:LEU:HD12	1:C:395:LEU:N	2.33	0.43
1:D:538:GLU:HG2	1:D:539:ILE:N	2.32	0.43
1:E:496:PRO:HG3	1:E:568:LEU:HB2	2.00	0.43
1:F:281:PHE:CE2	1:F:296:ILE:HG12	2.53	0.43
1:F:390:LYS:HE3	1:F:420:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:CYS:HA	1:B:98:ASN:O	2.17	0.43
1:B:449:THR:HG22	1:B:450:LYS:N	2.33	0.43
1:E:38:PRO:HD3	6:E:2169:HOH:O	2.18	0.43
1:E:82:HIS:O	1:E:95:LEU:HA	2.19	0.43
1:F:266:PRO:HB2	1:F:288:SER:HB2	2.00	0.43
1:F:290:THR:HG22	1:F:318:GLU:CA	2.48	0.43
1:F:433:TYR:CG	1:F:434:ALA:N	2.86	0.43
1:A:95:LEU:HD23	1:A:95:LEU:C	2.43	0.43
1:B:481:ILE:HD12	1:B:490:TYR:CE1	2.52	0.43
1:C:61:ASN:HD21	1:C:548:THR:HG21	1.81	0.43
1:C:75:ASN:HB2	1:D:53:SER:OG	2.18	0.43
1:D:109:ARG:NH2	1:D:112:ILE:CD1	2.81	0.43
1:D:363:TYR:CD1	1:D:364:ILE:HG13	2.54	0.43
1:D:454:GLU:HG3	6:D:2069:HOH:O	2.19	0.43
1:D:515:ILE:HG21	1:D:539:ILE:HD13	2.00	0.43
1:E:67:LEU:HD23	1:E:118:ILE:HD13	1.99	0.43
1:E:288:SER:C	1:E:290:THR:H	2.27	0.43
1:F:109:ARG:HB3	1:F:111:ASP:OD1	2.19	0.43
1:A:166:MET:HG2	1:A:182:ILE:HA	1.99	0.43
1:A:456:ASN:C	1:A:456:ASN:ND2	2.75	0.43
1:C:188:ASP:HB3	1:C:202:THR:OG1	2.19	0.43
1:C:210:VAL:HG13	1:C:211:ASP:N	2.33	0.43
1:D:365:ARG:HG3	1:D:365:ARG:HH11	1.83	0.43
1:E:61:ASN:HD21	1:E:548:THR:HG22	1.83	0.43
1:E:302:LEU:HD22	1:E:312:THR:HG21	1.99	0.43
1:A:83:ILE:HG22	1:A:440:ILE:HD13	1.99	0.43
1:B:562:ASN:HD22	1:B:562:ASN:N	2.17	0.43
1:F:48:VAL:H	1:F:50:ASN:ND2	2.17	0.43
1:F:210:VAL:HG13	1:F:211:ASP:N	2.34	0.43
1:F:339:PHE:CE1	1:F:373:GLN:HB3	2.54	0.43
1:A:181:VAL:HG22	1:A:251:VAL:CG2	2.49	0.43
1:A:470:ASP:HB3	1:A:481:ILE:CD1	2.47	0.43
1:C:85:MET:CE	1:C:134:LYS:HG2	2.48	0.43
1:D:150:PRO:HG2	1:D:153:ASN:HA	2.01	0.43
1:E:37:VAL:HG21	1:E:441:LEU:HD22	2.00	0.43
1:E:505:VAL:HG23	1:E:578:VAL:HG22	1.99	0.43
1:F:266:PRO:HB2	1:F:288:SER:CB	2.49	0.43
1:F:268:ASN:HB2	1:F:287:LEU:HD12	2.01	0.43
1:A:265:VAL:HA	1:A:266:PRO:HD3	1.87	0.43
1:A:392:LEU:HB2	1:A:419:ILE:HD13	2.01	0.43
1:B:495:ALA:HB3	6:B:2264:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:VAL:HA	1:C:249:PRO:HD3	1.88	0.43
1:D:135:VAL:HA	1:D:136:PRO:C	2.44	0.43
1:D:286:LYS:O	1:D:323:PRO:HD2	2.18	0.43
1:F:77:ASP:CG	1:F:79:HIS:HE2	2.26	0.43
1:F:366:GLN:HG2	1:F:367:LYS:N	2.34	0.43
1:C:43:LEU:O	1:D:411:PRO:HB3	2.19	0.43
1:E:180:GLN:NE2	6:E:2081:HOH:O	2.48	0.43
1:E:282:ILE:HD12	1:E:328:PHE:CE2	2.54	0.43
1:B:295:ALA:HB2	1:B:314:VAL:HG21	2.00	0.43
1:C:152:PRO:HG2	1:C:154:ASP:OD2	2.18	0.43
1:D:339:PHE:CE1	1:D:373:GLN:HB3	2.54	0.43
1:E:315:ALA:HA	1:E:356:TYR:CG	2.54	0.43
1:E:494:VAL:HG13	1:E:518:LEU:HB2	2.00	0.43
1:E:521:VAL:HB	1:E:524:VAL:HG21	2.01	0.43
1:B:370:VAL:HG11	1:B:374:PRO:HG3	2.00	0.42
1:D:433:TYR:CG	1:D:434:ALA:N	2.87	0.42
1:D:470:ASP:HB3	1:D:481:ILE:CD1	2.49	0.42
1:E:531:VAL:HG11	1:F:125:GLN:CG	2.48	0.42
1:F:75:ASN:ND2	1:F:102:ASN:HD21	2.17	0.42
1:F:286:LYS:N	1:F:323:PRO:HG2	2.32	0.42
1:F:457:ASP:HA	1:F:458:PRO:HD3	1.81	0.42
1:F:504:LYS:HG2	1:F:577:LEU:HB2	2.01	0.42
1:B:117:LYS:HB2	1:B:175:MET:HG3	2.01	0.42
1:D:491:MET:HB2	1:D:515:ILE:HD13	2.01	0.42
1:E:494:VAL:O	1:E:495:ALA:C	2.62	0.42
1:E:558:TRP:CE2	1:F:147:PHE:HB3	2.54	0.42
1:B:77:ASP:CG	1:B:79:HIS:HE2	2.26	0.42
1:C:478:ASN:ND2	1:C:492:THR:HG22	2.33	0.42
1:C:494:VAL:O	1:C:495:ALA:C	2.62	0.42
1:A:277:ASP:OD1	1:A:279:LYS:HG2	2.18	0.42
1:A:540:SER:HB3	1:A:541:PRO:CD	2.49	0.42
1:C:67:LEU:HD23	1:C:118:ILE:HD12	2.00	0.42
1:C:200:THR:HG22	1:C:225:VAL:HG22	2.01	0.42
1:C:376:HIS:HB2	1:C:437:HIS:O	2.20	0.42
1:E:56:GLY:O	1:E:60:THR:HG23	2.19	0.42
1:A:35:LEU:HD22	1:A:42:GLU:HA	2.01	0.42
1:B:371:GLN:C	1:B:372:TYR:CG	2.96	0.42
1:C:456:ASN:H	1:C:456:ASN:ND2	2.16	0.42
1:D:275:SER:HA	1:D:276:PRO:HD3	1.92	0.42
1:D:453:TYR:CD1	1:D:543:GLN:HB2	2.55	0.42
1:F:548:THR:HG22	6:F:2026:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASN:HD22	1:B:50:ASN:N	2.00	0.42
1:B:452:ILE:CD1	1:B:542:GLN:HG3	2.49	0.42
1:C:135:VAL:HA	1:C:136:PRO:C	2.44	0.42
1:D:540:SER:HB3	1:D:541:PRO:HD2	2.02	0.42
1:F:295:ALA:HB2	1:F:314:VAL:CG2	2.49	0.42
1:F:495:ALA:CA	6:F:2182:HOH:O	2.67	0.42
1:B:141:VAL:HB	1:B:170:ILE:HB	2.02	0.42
1:C:282:ILE:HD12	1:C:328:PHE:CE2	2.55	0.42
1:D:316:GLU:N	1:D:317:PRO:CD	2.83	0.42
1:F:363:TYR:CE1	1:F:364:ILE:HG13	2.54	0.42
1:B:370:VAL:HG13	1:B:415:GLN:HE21	1.85	0.42
1:C:113:MET:HG3	1:D:406:VAL:O	2.20	0.42
1:C:269:PRO:HA	1:C:284:ASN:O	2.19	0.42
1:C:282:ILE:HG23	1:C:291:VAL:CG1	2.50	0.42
1:C:553:LYS:HB2	1:C:554:PRO:HD2	2.01	0.42
1:D:87:ASP:N	1:D:136:PRO:O	2.51	0.42
1:D:125:GLN:HG3	1:D:149:ILE:HD13	2.01	0.42
1:D:456:ASN:HD22	1:D:456:ASN:N	2.15	0.42
1:E:75:ASN:HD22	1:E:75:ASN:N	2.17	0.42
1:E:575:ARG:HD3	6:E:2223:HOH:O	2.19	0.42
1:F:77:ASP:HB2	6:F:2040:HOH:O	2.19	0.42
1:F:200:THR:HG22	1:F:225:VAL:HG22	2.00	0.42
1:A:18:ASP:HB3	1:A:37:VAL:O	2.20	0.42
1:A:47:PRO:HA	1:A:50:ASN:HD21	1.85	0.42
1:B:119:THR:OG1	1:B:175:MET:HE3	2.19	0.42
1:F:262:TYR:CD1	1:F:262:TYR:N	2.88	0.42
1:F:538:GLU:HG2	1:F:539:ILE:N	2.34	0.42
1:A:372:TYR:O	1:A:396:SER:HB3	2.20	0.42
1:A:492:THR:HG22	1:A:499:GLY:HA3	2.01	0.42
1:A:520:MET:HB2	6:A:2308:HOH:O	2.19	0.42
1:A:537:MET:CE	1:A:547:VAL:HG12	2.49	0.42
1:C:205:ASN:OD1	1:C:208:ARG:N	2.53	0.42
1:D:368:LEU:HD23	1:D:369:ASP:N	2.34	0.42
1:D:371:GLN:CG	1:D:402:ARG:HD2	2.48	0.42
1:E:272:LEU:C	1:E:272:LEU:HD23	2.44	0.42
1:B:342:SER:HA	1:B:374:PRO:HD3	2.02	0.41
1:B:344:VAL:HG21	1:B:394:VAL:CG2	2.50	0.41
1:C:137:LYS:HG3	1:C:139:ASN:ND2	2.35	0.41
1:D:381:LEU:HD21	1:D:446:GLN:HE22	1.85	0.41
1:E:566:HIS:ND1	1:E:567:ALA:N	2.68	0.41
1:F:263:ILE:O	1:F:265:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:HIS:HA	1:A:77:ASP:HA	2.02	0.41
1:D:137:LYS:HG3	1:D:139:ASN:ND2	2.36	0.41
1:E:528:PHE:CD2	1:E:537:MET:HE2	2.56	0.41
1:C:451:LYS:HE2	1:D:410:HIS:CE1	2.54	0.41
1:C:562:ASN:C	1:C:562:ASN:HD22	2.28	0.41
1:E:512:THR:HG22	1:E:514:TYR:CE1	2.56	0.41
1:E:568:LEU:HD13	1:F:212:LEU:HD21	2.01	0.41
1:F:282:ILE:HD12	1:F:328:PHE:CE2	2.56	0.41
1:B:49:PHE:CZ	1:B:99:ASP:HB2	2.56	0.41
1:B:495:ALA:N	6:B:2265:HOH:O	2.53	0.41
1:C:365:ARG:HG3	1:C:365:ARG:HH11	1.85	0.41
1:C:372:TYR:HE2	1:C:402:ARG:HG2	1.84	0.41
1:C:568:LEU:HD21	1:D:287:LEU:HD21	2.00	0.41
1:E:494:VAL:HG22	6:E:2205:HOH:O	2.19	0.41
1:F:32:VAL:HG23	1:F:48:VAL:HG21	2.02	0.41
1:C:308:GLU:O	1:C:311:ASP:HB2	2.20	0.41
1:D:265:VAL:CG1	1:D:266:PRO:HD2	2.49	0.41
1:E:562:ASN:HD22	1:E:562:ASN:N	2.17	0.41
1:F:130:LEU:C	1:F:130:LEU:HD23	2.44	0.41
1:A:518:LEU:HD13	6:A:2282:HOH:O	2.20	0.41
1:B:371:GLN:CG	1:B:402:ARG:HD2	2.51	0.41
1:C:327:THR:HG22	1:C:377:ASN:ND2	2.35	0.41
1:D:57:TRP:CZ2	1:D:115:THR:HB	2.55	0.41
1:D:376:HIS:CE1	1:D:438:ASP:HB2	2.56	0.41
1:A:78:CYS:HB2	1:A:97:ILE:HG12	2.02	0.41
1:A:538:GLU:OE2	1:B:409:LEU:HG	2.21	0.41
1:A:540:SER:HB3	1:A:541:PRO:HD2	2.02	0.41
1:C:130:LEU:HA	1:C:142:PHE:O	2.21	0.41
1:C:363:TYR:CE1	1:C:364:ILE:HG13	2.55	0.41
1:D:78:CYS:HB2	1:D:97:ILE:CD1	2.51	0.41
1:D:127:ILE:HA	1:D:144:ASN:O	2.21	0.41
1:D:308:GLU:O	1:D:311:ASP:HB2	2.20	0.41
1:D:433:TYR:O	1:D:434:ALA:C	2.63	0.41
1:A:174:THR:O	1:A:175:MET:HB2	2.20	0.41
1:A:575:ARG:NH2	1:B:158:PHE:O	2.54	0.41
1:B:261:ARG:HA	6:B:2151:HOH:O	2.19	0.41
1:B:513:VAL:O	1:B:546:SER:HA	2.21	0.41
1:C:107:ARG:NH1	1:C:116:ASP:OD2	2.48	0.41
1:D:35:LEU:CD2	1:D:42:GLU:HA	2.51	0.41
1:D:75:ASN:HD22	1:D:75:ASN:N	2.17	0.41
1:D:492:THR:HG22	1:D:499:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:ARG:HB3	1:E:111:ASP:OD1	2.20	0.41
1:F:186:ASN:ND2	1:F:186:ASN:C	2.78	0.41
1:F:354:LYS:O	1:F:359:ASP:HB2	2.20	0.41
1:A:11:HIS:HB3	6:A:2001:HOH:O	2.21	0.41
1:A:410:HIS:CE1	1:B:451:LYS:HE3	2.55	0.41
1:B:117:LYS:CB	1:B:175:MET:HG3	2.51	0.41
1:B:470:ASP:HB3	1:B:481:ILE:CD1	2.43	0.41
1:C:49:PHE:CZ	1:C:99:ASP:HB2	2.56	0.41
1:C:95:LEU:HD22	1:C:108:ILE:HD12	2.03	0.41
1:C:287:LEU:HD21	1:D:568:LEU:HD21	2.03	0.41
1:D:37:VAL:CG1	1:D:38:PRO:HA	2.51	0.41
1:D:180:GLN:HG3	1:D:248:VAL:HG11	2.02	0.41
1:D:266:PRO:HB2	1:D:288:SER:OG	2.20	0.41
1:E:61:ASN:ND2	1:E:548:THR:HG22	2.35	0.41
1:E:371:GLN:HG2	1:E:402:ARG:HD2	2.02	0.41
1:F:204:TYR:CD1	1:F:204:TYR:C	2.98	0.41
1:F:361:VAL:HG12	1:F:362:ASN:N	2.36	0.41
1:F:449:THR:HB	6:F:2150:HOH:O	2.20	0.41
1:C:366:GLN:HG2	1:C:367:LYS:N	2.36	0.41
1:C:435:GLU:HA	1:C:436:PRO:HD2	2.03	0.41
1:D:282:ILE:HD12	1:D:328:PHE:CE2	2.56	0.41
1:D:295:ALA:HB2	1:D:314:VAL:CG2	2.51	0.41
1:D:321:LEU:HB3	1:D:340:ILE:HD12	2.02	0.41
1:F:37:VAL:HG21	1:F:441:LEU:HD22	2.03	0.41
1:B:291:VAL:O	1:B:316:GLU:HA	2.21	0.40
1:C:27:GLY:O	1:C:77:ASP:HA	2.21	0.40
1:C:57:TRP:CH2	1:C:115:THR:HB	2.56	0.40
1:C:207:GLU:HG3	1:C:218:ASN:ND2	2.36	0.40
1:C:433:TYR:CG	1:C:434:ALA:N	2.88	0.40
1:D:109:ARG:HD2	1:D:111:ASP:OD1	2.20	0.40
1:D:155:GLY:HA2	1:D:158:PHE:CE1	2.56	0.40
1:E:130:LEU:C	1:E:130:LEU:HD23	2.45	0.40
1:F:268:ASN:O	1:F:286:LYS:HD3	2.20	0.40
1:F:325:HIS:CD2	1:F:376:HIS:HA	2.56	0.40
1:F:344:VAL:HG21	1:F:394:VAL:CG2	2.51	0.40
1:F:376:HIS:HB2	1:F:437:HIS:O	2.21	0.40
1:A:297:ASP:HB2	6:A:2178:HOH:O	2.20	0.40
1:B:365:ARG:HG3	1:B:365:ARG:HH11	1.86	0.40
1:B:478:ASN:HA	1:B:490:TYR:O	2.21	0.40
1:D:135:VAL:HG13	1:D:136:PRO:HA	2.03	0.40
1:E:151:GLN:HA	1:E:152:PRO:HA	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:CYS:HA	1:F:98:ASN:O	2.21	0.40
1:F:343:GLN:HE22	1:F:367:LYS:HD3	1.82	0.40
1:F:494:VAL:HG22	6:F:2186:HOH:O	2.22	0.40
1:A:212:LEU:HD21	1:B:568:LEU:HD13	2.03	0.40
1:A:514:TYR:CD2	1:A:546:SER:HB3	2.56	0.40
1:B:174:THR:CG2	1:B:176:ASP:OD2	2.69	0.40
1:B:344:VAL:HG21	1:B:394:VAL:HG21	2.03	0.40
1:C:147:PHE:HB3	1:D:558:TRP:CE2	2.56	0.40
1:C:363:TYR:CD1	1:C:364:ILE:HG13	2.57	0.40
1:C:412:GLU:HG3	1:C:436:PRO:HD2	2.02	0.40
1:E:67:LEU:HD23	1:E:118:ILE:CD1	2.51	0.40
1:F:39:SER:O	1:F:40:MET:HB2	2.22	0.40
1:C:316:GLU:N	1:C:317:PRO:CD	2.84	0.40
1:E:100:LYS:HG3	1:E:126:ALA:HB1	2.04	0.40
1:A:189:ASN:O	1:A:201:SER:HA	2.21	0.40
1:A:200:THR:HG21	1:A:225:VAL:HG22	2.01	0.40
1:B:130:LEU:C	1:B:130:LEU:HD23	2.47	0.40
1:B:308:GLU:O	1:B:311:ASP:HB2	2.21	0.40
1:C:342:SER:HA	1:C:374:PRO:CD	2.49	0.40
1:E:328:PHE:CD1	1:E:328:PHE:N	2.89	0.40
1:F:533:HIS:O	1:F:535:VAL:HG23	2.21	0.40
1:F:548:THR:HG21	6:F:2025:HOH:O	2.19	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	570/581 (98%)	532 (93%)	31 (5%)	7 (1%)	10	16
1	B	570/581 (98%)	527 (92%)	35 (6%)	8 (1%)	9	13
1	C	570/581 (98%)	521 (91%)	41 (7%)	8 (1%)	9	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	570/581 (98%)	517 (91%)	44 (8%)	9 (2%)	7	11
1	E	570/581 (98%)	519 (91%)	47 (8%)	4 (1%)	18	28
1	F	570/581 (98%)	519 (91%)	45 (8%)	6 (1%)	11	18
All	All	3420/3486 (98%)	3135 (92%)	243 (7%)	42 (1%)	10	16

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	LYS
1	A	495	ALA
1	B	267	LYS
1	C	267	LYS
1	D	267	LYS
1	D	495	ALA
1	E	267	LYS
1	F	267	LYS
1	F	495	ALA
1	B	495	ALA
1	C	286	LYS
1	C	495	ALA
1	E	286	LYS
1	E	495	ALA
1	F	359	ASP
1	A	286	LYS
1	A	434	ALA
1	B	286	LYS
1	D	434	ALA
1	A	435	GLU
1	B	217	ARG
1	B	400	LYS
1	B	434	ALA
1	C	434	ALA
1	D	400	LYS
1	F	434	ALA
1	F	435	GLU
1	B	435	GLU
1	C	435	GLU
1	D	286	LYS
1	D	435	GLU
1	E	435	GLU
1	A	359	ASP

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Mol	Chain	Res	Type
1	C	217	ARG
1	D	373	GLN
1	F	286	LYS
1	C	289	PRO
1	D	496	PRO
1	C	373	GLN
1	A	289	PRO
1	B	373	GLN
1	D	289	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	491/497 (99%)	474 (96%)	17 (4%)	32	53
1	B	491/497 (99%)	471 (96%)	20 (4%)	27	46
1	C	491/497 (99%)	476 (97%)	15 (3%)	35	57
1	D	491/497 (99%)	476 (97%)	15 (3%)	35	57
1	E	491/497 (99%)	473 (96%)	18 (4%)	30	51
1	F	491/497 (99%)	474 (96%)	17 (4%)	32	53
All	All	2946/2982 (99%)	2844 (96%)	102 (4%)	32	53

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	75	ASN
1	A	107	ARG
1	A	124	VAL
1	A	186	ASN
1	A	210	VAL
1	A	212	LEU
1	A	291	VAL
1	A	304	GLU

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Mol	Chain	Res	Type
1	A	359	ASP
1	A	368	LEU
1	A	409	LEU
1	A	451	LYS
1	A	456	ASN
1	A	548	THR
1	A	562	ASN
1	A	563	TRP
1	B	50	ASN
1	B	75	ASN
1	B	103	THR
1	B	124	VAL
1	B	143	CYS
1	B	186	ASN
1	B	212	LEU
1	B	291	VAL
1	B	304	GLU
1	B	359	ASP
1	B	368	LEU
1	B	371	GLN
1	B	409	LEU
1	B	452	ILE
1	B	456	ASN
1	B	492	THR
1	B	539	ILE
1	B	548	THR
1	B	562	ASN
1	B	563	TRP
1	C	50	ASN
1	C	75	ASN
1	C	124	VAL
1	C	186	ASN
1	C	212	LEU
1	C	359	ASP
1	C	360	ARG
1	C	371	GLN
1	C	373	GLN
1	C	409	LEU
1	C	456	ASN
1	C	539	ILE
1	C	548	THR
1	C	562	ASN

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Mol	Chain	Res	Type
1	C	563	TRP
1	D	11	HIS
1	D	50	ASN
1	D	75	ASN
1	D	103	THR
1	D	124	VAL
1	D	186	ASN
1	D	212	LEU
1	D	359	ASP
1	D	371	GLN
1	D	373	GLN
1	D	409	LEU
1	D	456	ASN
1	D	548	THR
1	D	562	ASN
1	D	563	TRP
1	E	50	ASN
1	E	75	ASN
1	E	124	VAL
1	E	186	ASN
1	E	212	LEU
1	E	291	VAL
1	E	343	GLN
1	E	359	ASP
1	E	368	LEU
1	E	409	LEU
1	E	451	LYS
1	E	456	ASN
1	E	541	PRO
1	E	548	THR
1	E	561	CYS
1	E	562	ASN
1	E	563	TRP
1	E	564	PHE
1	F	50	ASN
1	F	75	ASN
1	F	103	THR
1	F	124	VAL
1	F	186	ASN
1	F	212	LEU
1	F	291	VAL
1	F	371	GLN

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Mol	Chain	Res	Type
1	F	373	GLN
1	F	409	LEU
1	F	452	ILE
1	F	456	ASN
1	F	492	THR
1	F	539	ILE
1	F	548	THR
1	F	562	ASN
1	F	563	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	71	GLN
1	A	72	GLN
1	A	75	ASN
1	A	98	ASN
1	A	120	HIS
1	A	125	GLN
1	A	139	ASN
1	A	144	ASN
1	A	151	GLN
1	A	180	GLN
1	A	186	ASN
1	A	189	ASN
1	A	218	ASN
1	A	343	GLN
1	A	362	ASN
1	A	366	GLN
1	A	371	GLN
1	A	373	GLN
1	A	410	HIS
1	A	415	GLN
1	A	446	GLN
1	A	456	ASN
1	A	517	ASN
1	A	542	GLN
1	A	543	GLN
1	A	562	ASN
1	B	50	ASN
1	B	71	GLN

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Mol	Chain	Res	Type
1	B	75	ASN
1	B	98	ASN
1	B	125	GLN
1	B	139	ASN
1	B	144	ASN
1	B	151	GLN
1	B	186	ASN
1	B	189	ASN
1	B	218	ASN
1	B	343	GLN
1	B	362	ASN
1	B	366	GLN
1	B	371	GLN
1	B	373	GLN
1	B	415	GLN
1	B	446	GLN
1	B	456	ASN
1	B	543	GLN
1	B	562	ASN
1	C	50	ASN
1	C	61	ASN
1	C	71	GLN
1	C	72	GLN
1	C	75	ASN
1	C	98	ASN
1	C	120	HIS
1	C	125	GLN
1	C	139	ASN
1	C	144	ASN
1	C	151	GLN
1	C	186	ASN
1	C	218	ASN
1	C	273	ASN
1	C	284	ASN
1	C	333	ASN
1	C	343	GLN
1	C	362	ASN
1	C	366	GLN
1	C	371	GLN
1	C	413	ASN
1	C	415	GLN
1	C	446	GLN

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Mol	Chain	Res	Type
1	C	456	ASN
1	C	466	GLN
1	C	543	GLN
1	C	562	ASN
1	D	50	ASN
1	D	61	ASN
1	D	71	GLN
1	D	72	GLN
1	D	75	ASN
1	D	98	ASN
1	D	120	HIS
1	D	125	GLN
1	D	139	ASN
1	D	144	ASN
1	D	151	GLN
1	D	186	ASN
1	D	189	ASN
1	D	218	ASN
1	D	333	ASN
1	D	343	GLN
1	D	362	ASN
1	D	366	GLN
1	D	371	GLN
1	D	413	ASN
1	D	415	GLN
1	D	446	GLN
1	D	456	ASN
1	D	542	GLN
1	D	543	GLN
1	D	562	ASN
1	E	50	ASN
1	E	61	ASN
1	E	71	GLN
1	E	72	GLN
1	E	75	ASN
1	E	98	ASN
1	E	125	GLN
1	E	139	ASN
1	E	144	ASN
1	E	151	GLN
1	E	180	GLN
1	E	186	ASN

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Mol	Chain	Res	Type
1	E	189	ASN
1	E	284	ASN
1	E	333	ASN
1	E	343	GLN
1	E	362	ASN
1	E	366	GLN
1	E	371	GLN
1	E	373	GLN
1	E	410	HIS
1	E	415	GLN
1	E	446	GLN
1	E	456	ASN
1	E	542	GLN
1	E	543	GLN
1	E	562	ASN
1	F	11	HIS
1	F	50	ASN
1	F	61	ASN
1	F	71	GLN
1	F	72	GLN
1	F	75	ASN
1	F	98	ASN
1	F	125	GLN
1	F	139	ASN
1	F	144	ASN
1	F	151	GLN
1	F	186	ASN
1	F	343	GLN
1	F	362	ASN
1	F	366	GLN
1	F	377	ASN
1	F	415	GLN
1	F	446	GLN
1	F	456	ASN
1	F	542	GLN
1	F	543	GLN
1	F	562	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 18 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CUZ	C	801	1,6	0,9,9	-	-	-		
2	CUA	B	701	-	0,1,1	-	-	-		
3	CUZ	F	801	1,6	0,9,9	-	-	-		
3	CUZ	B	801	1,6	0,9,9	-	-	-		
2	CUA	A	701	-	0,1,1	-	-	-		
2	CUA	D	701	1	0,1,1	-	-	-		
3	CUZ	E	801	1,6	0,9,9	-	-	-		
2	CUA	F	701	1	0,1,1	-	-	-		
3	CUZ	A	801	1,6	0,9,9	-	-	-		
3	CUZ	D	801	1,6	0,9,9	-	-	-		
2	CUA	C	701	1	0,1,1	-	-	-		
2	CUA	E	701	1	0,1,1	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	801	CUZ	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	572/581 (98%)	0.10	7 (1%) 76 73	31, 52, 70, 91	3 (0%)
1	B	572/581 (98%)	0.08	9 (1%) 70 66	32, 52, 71, 91	3 (0%)
1	C	572/581 (98%)	0.56	18 (3%) 51 47	36, 60, 77, 91	3 (0%)
1	D	572/581 (98%)	0.44	12 (2%) 63 59	36, 58, 75, 92	3 (0%)
1	E	572/581 (98%)	0.35	26 (4%) 38 34	35, 54, 71, 89	3 (0%)
1	F	572/581 (98%)	0.53	33 (5%) 29 25	34, 58, 75, 91	3 (0%)
All	All	3432/3486 (98%)	0.34	105 (3%) 51 47	31, 56, 74, 92	18 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	435	GLU	4.8
1	D	573	VAL	4.6
1	B	573	VAL	4.1
1	E	573	VAL	4.0
1	F	269	PRO	3.9
1	E	574	GLY	3.7
1	A	353	ILE	3.6
1	F	259	PHE	3.6
1	B	434	ALA	3.5
1	C	299	LEU	3.4
1	F	200	THR	3.4
1	B	11	HIS	3.3
1	B	449	THR	3.2
1	F	485	ASN	3.1
1	E	559	TYR	3.1
1	A	485	ASN	3.1
1	F	573	VAL	3.0
1	E	578	VAL	2.9
1	A	434	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	164	TYR	2.8
1	B	361	VAL	2.8
1	E	545	ALA	2.8
1	D	349	ILE	2.7
1	E	556	VAL	2.7
1	F	206	SER	2.7
1	F	186	ASN	2.7
1	F	132	LEU	2.7
1	E	434	ALA	2.7
1	E	464	ARG	2.7
1	E	474	LEU	2.6
1	F	224	VAL	2.6
1	A	10	ALA	2.6
1	C	10	ALA	2.6
1	D	353	ILE	2.6
1	E	485	ASN	2.6
1	F	434	ALA	2.6
1	F	495	ALA	2.6
1	D	280	TYR	2.6
1	C	314	VAL	2.6
1	F	484	GLY	2.6
1	C	573	VAL	2.6
1	C	349	ILE	2.5
1	D	413	ASN	2.5
1	E	377	ASN	2.5
1	F	483	ASP	2.5
1	F	205	ASN	2.5
1	E	493	SER	2.5
1	F	314	VAL	2.5
1	B	495	ALA	2.5
1	D	333	ASN	2.5
1	C	309	LEU	2.4
1	F	432	THR	2.4
1	E	577	LEU	2.4
1	C	198	TYR	2.4
1	B	200	THR	2.3
1	F	375	GLY	2.3
1	F	303	PHE	2.3
1	F	344	VAL	2.3
1	F	185	GLY	2.3
1	C	350	ALA	2.3
1	D	283	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	149	ILE	2.3
1	F	184	ASP	2.3
1	C	303	PHE	2.3
1	E	524	VAL	2.3
1	E	11	HIS	2.2
1	C	353	ILE	2.2
1	E	503	PHE	2.2
1	D	377	ASN	2.2
1	F	233	ALA	2.2
1	C	185	GLY	2.2
1	F	435	GLU	2.2
1	E	564	PHE	2.2
1	C	224	VAL	2.2
1	C	377	ASN	2.2
1	D	291	VAL	2.1
1	B	581	ALA	2.1
1	E	554	PRO	2.1
1	C	563	TRP	2.1
1	A	358	GLY	2.1
1	E	561	CYS	2.1
1	F	11	HIS	2.1
1	A	573	VAL	2.1
1	E	581	ALA	2.1
1	F	353	ILE	2.1
1	C	11	HIS	2.1
1	D	427	VAL	2.1
1	F	265	VAL	2.1
1	A	495	ALA	2.1
1	D	309	LEU	2.1
1	E	547	VAL	2.0
1	F	223	VAL	2.0
1	E	580	ALA	2.0
1	F	360	ARG	2.0
1	C	333	ASN	2.0
1	C	381	LEU	2.0
1	F	362	ASN	2.0
1	C	421	GLY	2.0
1	E	200	THR	2.0
1	E	558	TRP	2.0
1	E	498	TYR	2.0
1	F	204	TYR	2.0
1	D	325	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	148	VAL	2.0
1	E	174	THR	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
5	CL	D	902	1/1	0.92	0.12	71,71,71,71	0
4	CA	F	903	1/1	0.93	0.07	67,67,67,67	0
3	CUZ	D	801	5/5	0.94	0.07	59,61,62,64	0
3	CUZ	F	801	5/5	0.94	0.07	61,61,63,63	0
4	CA	D	903	1/1	0.95	0.08	70,70,70,70	0
5	CL	C	902	1/1	0.95	0.07	75,75,75,75	0
4	CA	F	901	1/1	0.95	0.05	67,67,67,67	0
5	CL	F	902	1/1	0.95	0.07	73,73,73,73	0
3	CUZ	C	801	5/5	0.96	0.06	62,65,66,67	0
4	CA	A	901	1/1	0.97	0.04	46,46,46,46	0
4	CA	C	903	1/1	0.97	0.04	63,63,63,63	0
3	CUZ	E	801	5/5	0.97	0.05	44,45,47,48	0
5	CL	E	902	1/1	0.97	0.09	46,46,46,46	0
3	CUZ	A	801	5/5	0.97	0.04	43,44,45,48	0
2	CUA	C	701	2/2	0.98	0.04	57,57,57,58	0
4	CA	E	903	1/1	0.98	0.03	47,47,47,47	0
3	CUZ	B	801	5/5	0.98	0.04	44,44,47,50	0
2	CUA	E	701	2/2	0.98	0.03	56,56,56,59	0
5	CL	B	902	1/1	0.98	0.08	43,43,43,43	0
4	CA	B	903	1/1	0.98	0.03	49,49,49,49	0
4	CA	C	901	1/1	0.98	0.03	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CUA	F	701	2/2	0.98	0.03	38,38,38,38	0
4	CA	D	901	1/1	0.98	0.03	64,64,64,64	0
2	CUA	D	701	2/2	0.99	0.04	54,54,54,57	0
5	CL	A	902	1/1	0.99	0.05	44,44,44,44	0
4	CA	A	903	1/1	0.99	0.02	41,41,41,41	0
4	CA	B	901	1/1	0.99	0.05	50,50,50,50	0
4	CA	E	901	1/1	0.99	0.03	41,41,41,41	0
2	CUA	B	701	2/2	0.99	0.02	37,37,37,38	0
2	CUA	A	701	2/2	0.99	0.02	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.