



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:31 PM UTC

PDB ID : 1YNT / pdb_00001ynt
Title : Structure of the monomeric form of T. gondii SAG1 surface antigen bound to a human Fab
Authors : Graille, M.; Stura, E.A.; Bossus, M.; Muller, B.H.; Letourneur, O.; Battail-Poirot, N.; Sibai, G.; Rolland, D.; Le Du, M.H.; Ducancel, F.
Deposited on : 2005-01-25
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

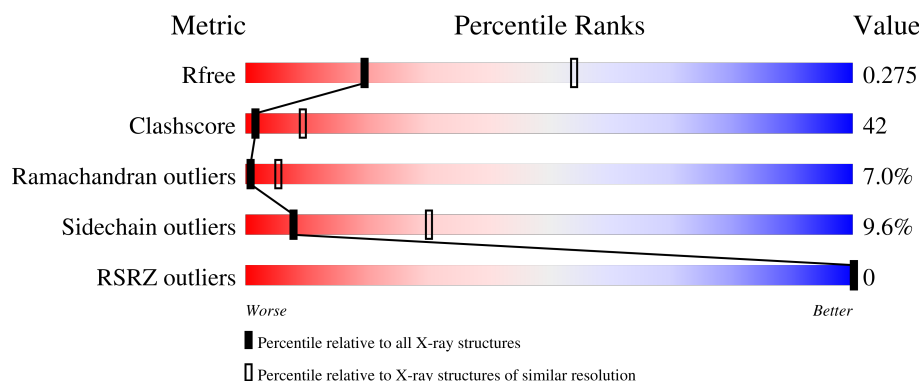
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

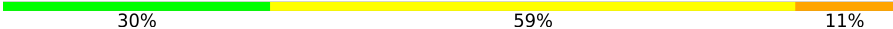
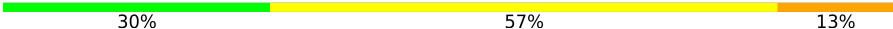
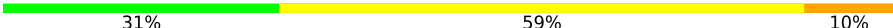
The reported resolution of this entry is 3.10 Å.

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



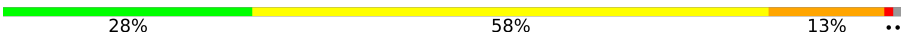
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	213	
1	C	213	
2	B	218	
2	D	218	
3	E	61	

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Mol	Chain	Length	Quality of chain
4	F	254	 30%56%13%..
4	G	254	 28%58%13%..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10802 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 4F11E12 Fab variable light chain region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1658	1027	280	346	5			
1	C	213	Total	C	N	O	S	0	0	0
			1658	1027	280	346	5			

- Molecule 2 is a protein called 4F11E12 Fab variable heavy chain region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1657	1048	269	332	8			
2	D	218	Total	C	N	O	S	0	0	0
			1657	1048	269	332	8			

- Molecule 3 is a protein called protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	61	Total	C	N	O	S	0	0	0
			476	302	76	97	1			

- Molecule 4 is a protein called Major surface antigen p30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	252	Total	C	N	O	S	0	0	0
			1847	1151	308	374	14			
4	G	252	Total	C	N	O	S	0	0	0
			1847	1151	308	374	14			

- Molecule 5 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cd	0	0
			1	1		

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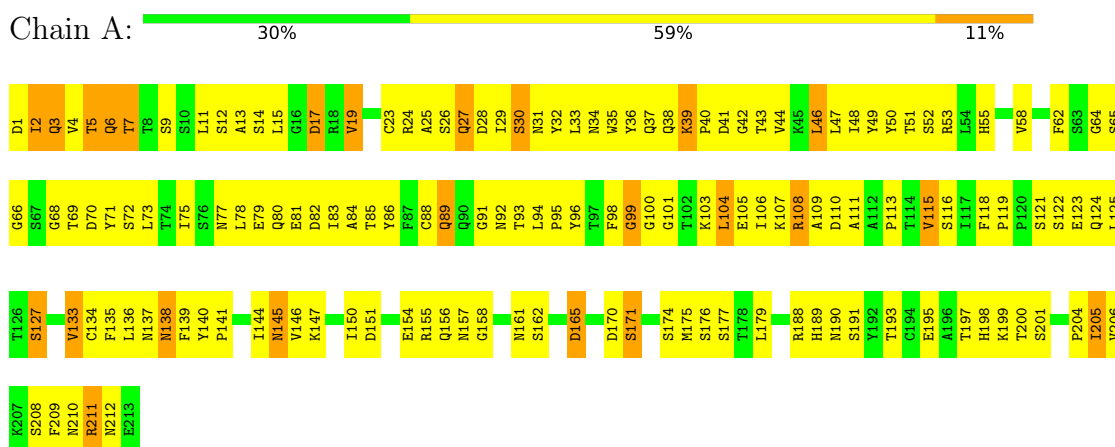
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cd	0	0
			1	1		

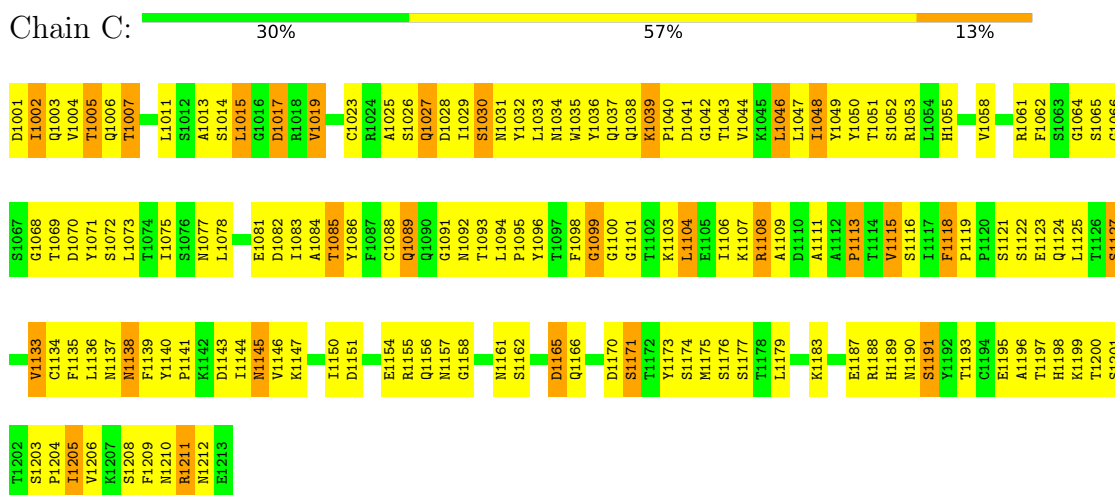
3 Residue-property plots

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

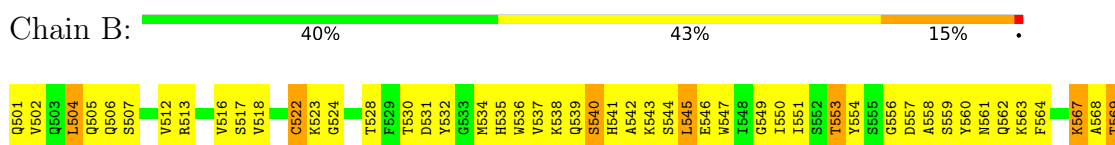
• Molecule 1: 4F11E12 Fab variable light chain region

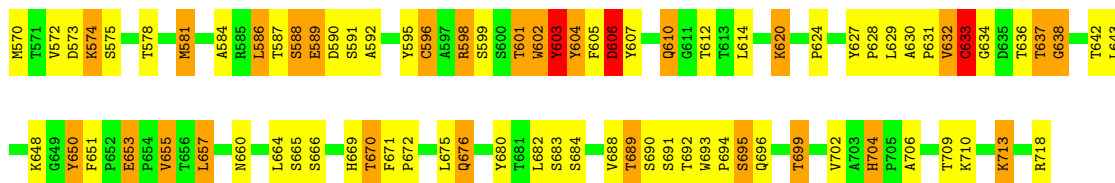


• Molecule 1: 4F11E12 Fab variable light chain region

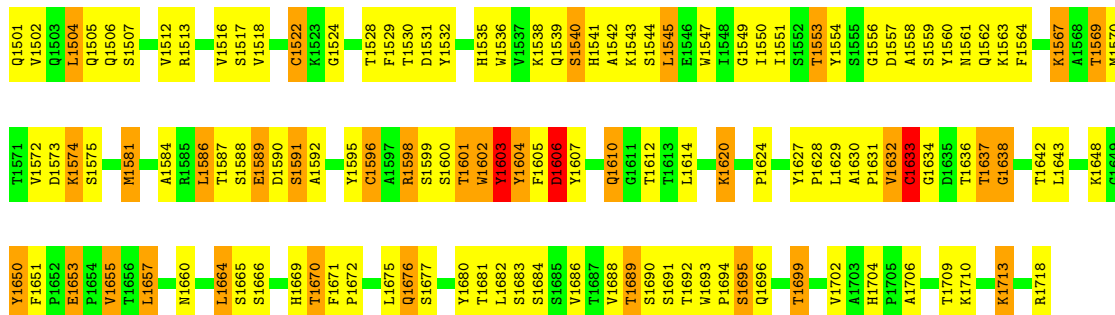


• Molecule 2: 4F11E12 Fab variable heavy chain region





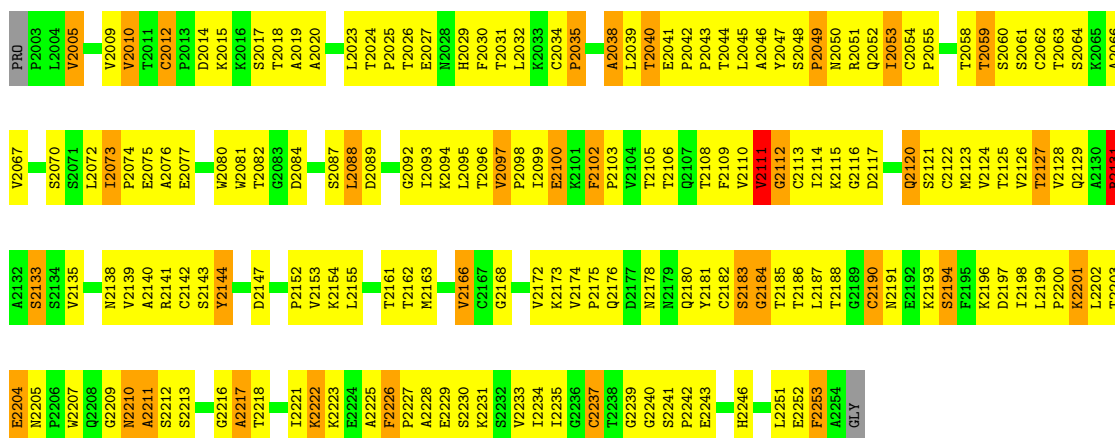
• Molecule 2: 4F11E12 Fab variable heavy chain region



• Molecule 3: protein L



• Molecule 4: Major surface antigen p30



• Molecule 4: Major surface antigen p30



L3202	S3133	S3070	PRD
T3203	S3134	S3071	P3003
E3204	V3135	L3072	L3004
N3205			V3005
W3207	N3138	I3073	V3009
Q3208	V3139	P3074	V3010
G3209	A3140	E3075	T3011
N3210	R3141	A3076	C3012
A3211	C3142	E3077	P3013
S3212	S3143		D3014
S3213	Y3144	W3080	K3015
	D3147	W3081	K3016
G3216		T3082	S3017
A3217	P3152	G3083	T3018
T3218	V3153	D3084	A3019
	K3154		
I3221	L3155	S3087	L3023
K3222	L3156	L3088	T3024
K3223	S3156	D3089	P3025
E3224	A3157		T3026
A3225	E3158	G3092	E3027
F3226		I3093	N3028
A3228	T3161	K3094	F3029
E3229	T3162	L3095	F3030
S3230	K3163	T3096	T3031
K3231		V3097	L3032
S3232	V3166	P3098	P3035
V3233	C3167	I3099	
I3234	G3168	E3100	A3038
I3235		K3101	L3039
G3236	V3172	F3102	T3040
C3237	K3173	P3103	E3041
T3238	V3174	V3104	P3042
G3239	P3175	T3105	P3043
S3241	Q3176	T3106	T3044
F3242	D3177	T3107	L3045
E3243	N3178	T3108	A3046
	N3179	F3109	Y3047
L3261	Q3180	V3110	S3048
E3262	Y3181	V3111	P3049
F3263	C3182	G3112	K3050
A3264	S3183	I3114	R3051
GLY	G3184	K3115	Q3052
	T3185	G3116	I3053
	T3186	D3117	C3054
	L3187		P3055
	T3188		
	G3189	Q3120	T3058
	C3190	S3121	T3059
	N3191	C3122	S3060
	K3192	M3123	S3061
	K3193	V3124	C3062
	E3194	T3125	T3063
	F3195	V3126	S3064
	K3196	T3127	K3065
	D3197	V3128	A3066
	T3198	Q3129	Y3067
	L3199	R3130	
	P3200	R3131	
	K3201	A3132	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.03Å 198.28Å 128.37Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-3.10) 96.6 (20.00-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.283 0.237 , 0.275	Depositor DCC
R_{free} test set	1579 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	71.2	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10802	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: CD

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	0.59	0/1692	1.07	14/2297 (0.6%)
1	C	0.59	0/1692	1.08	16/2297 (0.7%)
2	B	0.64	0/1700	1.15	23/2318 (1.0%)
2	D	0.65	0/1700	1.16	24/2318 (1.0%)
3	E	0.60	0/483	1.03	3/649 (0.5%)
4	F	0.41	0/1882	0.98	13/2568 (0.5%)
4	G	0.42	0/1882	0.98	12/2568 (0.5%)
All	All	0.56	0/11031	1.07	105/15015 (0.7%)

There are no bond length outliers.

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1158	GLY	N-CA-C	-9.65	101.82	115.43
1	A	158	GLY	N-CA-C	-9.54	101.97	115.43
2	D	1602	TRP	N-CA-C	8.34	120.06	110.97
2	B	602	TRP	N-CA-C	7.94	119.63	110.97
2	B	553	THR	N-CA-C	7.39	121.22	111.75
2	D	1696	GLN	N-CA-C	-7.33	100.65	110.55
2	B	653	GLU	N-CA-C	7.31	125.96	109.81
2	D	1553	THR	N-CA-C	7.18	120.94	111.75
2	D	1653	GLU	N-CA-C	7.14	125.60	109.81
4	G	3144	TYR	N-CA-C	7.01	119.86	110.88
2	D	1542	ALA	N-CA-C	-7.01	103.23	114.09
2	B	696	GLN	N-CA-C	-6.97	101.14	110.55
2	B	542	ALA	N-CA-C	-6.89	103.41	114.09
2	B	650	TYR	N-CA-C	6.57	119.80	110.14
4	F	2144	TYR	N-CA-C	6.46	119.15	110.88
4	G	3073	ILE	CA-C-N	6.32	127.73	119.84
4	G	3073	ILE	C-N-CA	6.32	127.73	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1540	SER	N-CA-C	-6.28	98.39	109.06
4	G	3012	CYS	N-CA-C	6.27	117.79	109.83
4	F	2012	CYS	N-CA-C	6.18	117.68	109.83
1	C	1115	VAL	N-CA-C	6.18	117.61	109.21
2	D	1650	TYR	N-CA-C	6.11	119.12	110.14
1	A	30	SER	N-CA-C	6.01	119.64	111.17
4	G	3059	THR	N-CA-C	-6.00	101.32	110.14
1	C	1030	SER	N-CA-C	5.99	119.62	111.17
4	G	3166	VAL	N-CA-C	5.99	112.61	106.21
4	F	2073	ILE	CA-C-N	5.98	127.32	119.84
4	F	2073	ILE	C-N-CA	5.98	127.32	119.84
4	F	2166	VAL	N-CA-C	5.95	112.57	106.21
2	B	603	TYR	N-CA-C	5.89	118.48	111.71
2	B	630	ALA	CA-C-N	5.85	127.15	119.84
2	B	630	ALA	C-N-CA	5.85	127.15	119.84
4	F	2097	VAL	N-CA-C	5.83	114.25	107.89
1	C	1145	ASN	N-CA-C	5.82	117.46	107.28
1	A	145	ASN	N-CA-C	5.80	117.06	107.20
4	G	3102	PHE	CA-C-N	5.76	125.67	119.85
4	G	3102	PHE	C-N-CA	5.76	125.67	119.85
1	A	39	LYS	CA-C-N	5.75	125.88	119.32
1	A	39	LYS	C-N-CA	5.75	125.88	119.32
2	D	1666	SER	N-CA-C	-5.75	101.78	110.28
2	D	1603	TYR	N-CA-C	5.74	118.31	111.71
1	A	133	VAL	N-CA-C	5.74	116.69	110.21
4	F	2059	THR	N-CA-C	-5.73	101.25	110.14
4	G	3097	VAL	N-CA-C	5.71	114.11	107.89
1	A	3	GLN	N-CA-C	5.69	119.06	110.64
1	C	1133	VAL	N-CA-C	5.65	116.59	110.21
1	A	115	VAL	N-CA-C	5.64	116.89	109.21
1	A	127	SER	N-CA-C	-5.64	106.44	113.38
1	A	165	ASP	N-CA-C	-5.62	103.29	110.53
2	D	1669	HIS	CB-CA-C	-5.61	103.77	110.94
1	C	1156	GLN	N-CA-C	5.60	120.61	113.55
2	D	1596	CYS	N-CA-C	-5.56	100.82	109.72
3	E	850	ALA	N-CA-C	-5.53	105.26	112.23
2	D	1556	GLY	N-CA-C	-5.52	107.63	115.30
4	F	2112	GLY	N-CA-C	5.50	121.05	112.31
4	F	2183	SER	N-CA-C	-5.49	106.25	113.12
1	A	157	ASN	N-CA-C	5.49	118.20	109.81
4	F	2102	PHE	CA-C-N	5.48	125.39	119.85
4	F	2102	PHE	C-N-CA	5.48	125.39	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	864	TYR	N-CA-C	5.48	118.48	109.72
2	B	556	GLY	N-CA-C	-5.44	107.76	115.43
2	D	1567	LYS	N-CA-C	-5.43	105.78	112.72
2	D	1677	SER	N-CA-C	-5.40	105.33	112.24
1	C	1203	SER	CA-C-N	5.39	125.56	119.90
1	C	1203	SER	C-N-CA	5.39	125.56	119.90
1	C	1157	ASN	N-CA-C	5.39	118.06	109.81
2	B	540	SER	N-CA-C	-5.38	99.17	108.69
4	G	3183	SER	N-CA-C	-5.35	106.44	113.12
2	B	669	HIS	CB-CA-C	-5.34	104.10	110.94
2	D	1586	LEU	N-CA-C	5.33	118.17	110.28
2	B	666	SER	N-CA-C	-5.30	102.43	110.28
2	D	1630	ALA	CA-C-N	5.30	126.47	119.84
2	D	1630	ALA	C-N-CA	5.30	126.47	119.84
2	B	596	CYS	N-CA-C	-5.29	101.25	109.72
2	B	567	LYS	N-CA-C	-5.28	105.92	112.93
4	G	3188	THR	N-CA-C	-5.26	105.44	111.07
1	C	1165	ASP	N-CA-C	-5.23	103.79	110.53
1	A	156	GLN	N-CA-C	5.21	120.11	113.55
2	B	586	LEU	N-CA-C	5.18	117.95	110.28
4	F	2188	THR	N-CA-C	-5.18	105.53	111.07
2	D	1545	LEU	N-CA-C	5.17	117.81	110.10
2	B	564	PHE	N-CA-C	5.17	119.22	113.02
1	C	1039	LYS	CA-C-N	5.14	126.27	119.84
1	C	1039	LYS	C-N-CA	5.14	126.27	119.84
1	C	1127	SER	N-CA-C	-5.14	106.70	113.17
2	B	545	LEU	N-CA-C	5.13	117.74	110.10
2	D	1589	GLU	N-CA-C	-5.13	106.87	113.23
1	C	1005	THR	N-CA-C	5.12	117.03	108.99
3	E	857	LEU	N-CA-C	-5.11	105.80	112.23
1	A	5	THR	N-CA-C	5.08	117.69	109.06
2	D	1600	SER	N-CA-C	-5.08	105.87	111.71
1	C	1118	PHE	CA-C-N	5.07	125.60	120.38
1	C	1118	PHE	C-N-CA	5.07	125.60	120.38
1	A	110	ASP	N-CA-C	-5.07	102.98	110.48
2	D	1591	SER	N-CA-C	-5.06	102.42	109.96
2	B	589	GLU	N-CA-C	-5.05	106.97	113.23
2	B	704	HIS	CA-C-N	5.04	125.07	119.32
2	B	704	HIS	C-N-CA	5.04	125.07	119.32
4	F	2142	CYS	N-CA-C	5.04	116.94	108.73
4	G	3142	CYS	N-CA-C	5.04	116.95	108.73
2	B	669	HIS	CA-C-N	-5.03	116.06	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	669	HIS	C-N-CA	-5.03	116.06	123.00
2	D	1564	PHE	N-CA-C	5.01	119.04	113.02
2	D	1540	SER	CA-C-N	-5.01	114.93	122.24
2	D	1540	SER	C-N-CA	-5.01	114.93	122.24

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	1658	0	1583	144	0
1	C	1658	0	1580	145	0
2	B	1657	0	1607	126	0
2	D	1657	0	1607	122	0
3	E	476	0	456	43	0
4	F	1847	0	1844	175	0
4	G	1847	0	1844	183	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
All	All	10802	0	10521	891	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 42.

All (891) 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)
4:G:3133:SER:HB3	4:G:3143:SER:H	1.14	1.11
4:F:2133:SER:HB3	4:F:2143:SER:H	1.14	1.08
2:D:1624:PRO:HB3	2:D:1650:TYR:HB3	1.35	1.05
2:B:624:PRO:HB3	2:B:650:TYR:HB3	1.36	1.02
1:C:1002:ILE:HG12	1:C:1002:ILE:O	1.59	1.01
1:A:34:ASN:HD22	1:A:89:GLN:NE2	1.60	0.98
1:A:2:ILE:HG12	1:A:2:ILE:O	1.60	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1034:ASN:HD22	1:C:1089:GLN:NE2	1.61	0.97
4:F:2121:SER:HB2	4:F:2123:MET:HE3	1.49	0.95
1:A:34:ASN:HD22	1:A:89:GLN:HE22	1.13	0.92
4:G:3183:SER:HB2	4:G:3191:ASN:HD22	1.34	0.92
2:D:1572:VAL:HG22	2:D:1573:ASP:H	1.35	0.92
2:B:572:VAL:HG22	2:B:573:ASP:H	1.33	0.91
4:G:3121:SER:HB2	4:G:3123:MET:HE3	1.51	0.91
2:D:1518:VAL:HG12	2:D:1586:LEU:HD11	1.53	0.91
4:F:2183:SER:HB2	4:F:2191:ASN:HD22	1.36	0.90
1:C:1034:ASN:HD22	1:C:1089:GLN:HE22	1.12	0.88
2:D:1536:TRP:CD2	2:D:1581:MET:HG3	2.08	0.88
1:C:1150:ILE:HD11	1:C:1179:LEU:HD21	1.56	0.87
2:B:536:TRP:CD2	2:B:581:MET:HG3	2.09	0.87
1:C:1205:ILE:HD13	1:C:1205:ILE:H	1.41	0.86
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.57	0.86
1:C:1091:GLY:HA3	2:D:1603:TYR:HB2	1.56	0.86
1:C:1017:ASP:O	1:C:1077:ASN:HA	1.75	0.86
2:B:518:VAL:HG12	2:B:586:LEU:HD11	1.59	0.85
1:A:91:GLY:HA3	2:B:603:TYR:HB2	1.59	0.85
4:G:3041:GLU:O	4:G:3043:PRO:HD3	1.77	0.84
3:E:876:ASN:O	3:E:877:ILE:HG13	1.78	0.84
4:G:3019:ALA:HB3	4:G:3124:VAL:HG22	1.60	0.83
4:F:2041:GLU:O	4:F:2043:PRO:HD3	1.78	0.83
1:C:1046:LEU:HD12	1:C:1055:HIS:HD2	1.43	0.83
2:D:1549:GLY:HA3	2:D:1570:MET:HE1	1.61	0.83
4:G:3010:VAL:HG11	4:G:3124:VAL:HG21	1.60	0.83
2:B:682:LEU:HD23	2:B:683:SER:N	1.94	0.83
1:A:17:ASP:O	1:A:77:ASN:HA	1.77	0.82
1:A:205:ILE:HD13	1:A:205:ILE:H	1.43	0.82
1:C:1085:THR:OG1	1:C:1103:LYS:HG2	1.80	0.82
2:D:1657:LEU:CD2	2:D:1702:VAL:HG22	2.09	0.82
4:F:2183:SER:HB2	4:F:2191:ASN:ND2	1.96	0.81
1:A:36:TYR:CE2	1:A:46:LEU:HD23	2.16	0.81
1:A:46:LEU:HD12	1:A:55:HIS:HD2	1.45	0.81
4:F:2019:ALA:HB3	4:F:2124:VAL:HG22	1.62	0.81
2:B:549:GLY:HA3	2:B:570:MET:HE1	1.63	0.81
2:B:657:LEU:CD2	2:B:702:VAL:HG22	2.11	0.81
2:D:1682:LEU:HD23	2:D:1683:SER:N	1.95	0.81
4:G:3183:SER:HB2	4:G:3191:ASN:ND2	1.95	0.81
4:F:2010:VAL:HG11	4:F:2124:VAL:HG21	1.61	0.81
4:G:3025:PRO:HA	4:G:3099:ILE:HD12	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2133:SER:HB3	4:F:2143:SER:N	1.95	0.80
1:C:1036:TYR:CE2	1:C:1046:LEU:HD23	2.15	0.80
1:C:1046:LEU:HD12	1:C:1055:HIS:CD2	2.16	0.80
4:F:2199:LEU:HD11	4:F:2227:PRO:HD3	1.63	0.80
4:F:2025:PRO:HA	4:F:2099:ILE:HD12	1.64	0.80
4:G:3199:LEU:HD11	4:G:3227:PRO:HD3	1.62	0.80
2:D:1516:VAL:HG12	2:D:1517:SER:N	1.98	0.79
1:A:49:TYR:O	1:A:53:ARG:HB2	1.82	0.79
4:G:3133:SER:HB3	4:G:3143:SER:N	1.95	0.78
1:A:46:LEU:HD12	1:A:55:HIS:CD2	2.16	0.78
1:A:26:SER:O	1:A:27:GLN:HB3	1.84	0.78
1:C:1088:CYS:O	1:C:1099:GLY:N	2.18	0.77
3:E:849:GLU:HG2	3:E:852:ARG:NH1	1.99	0.77
2:B:516:VAL:HG12	2:B:517:SER:N	1.99	0.77
1:C:1026:SER:O	1:C:1027:GLN:HB3	1.83	0.77
1:C:1049:TYR:O	1:C:1053:ARG:HB2	1.84	0.76
3:E:829:PHE:HZ	3:E:857:LEU:HD13	1.51	0.75
4:G:3156:SER:HB2	4:G:3254:ALA:HB3	1.67	0.75
1:A:9:SER:OG	3:E:840:LYS:HE2	1.87	0.75
4:G:3009:VAL:HG22	4:G:3031:THR:HB	1.69	0.74
2:D:1624:PRO:CB	2:D:1650:TYR:HB3	2.17	0.74
1:A:88:CYS:O	1:A:99:GLY:N	2.20	0.74
2:B:559:SER:HA	4:F:2050:ASN:HD21	1.53	0.73
4:G:3131:ARG:HA	4:G:3131:ARG:NE	2.05	0.72
1:C:1023:CYS:HB2	1:C:1035:TRP:CH2	2.25	0.72
1:A:193:THR:HG23	1:A:208:SER:HB3	1.71	0.71
4:F:2009:VAL:HG22	4:F:2031:THR:HB	1.71	0.71
1:C:1089:GLN:HB2	1:C:1098:PHE:CD1	2.25	0.71
2:B:688:VAL:HG12	2:B:689:THR:H	1.57	0.70
4:F:2201:LYS:HE3	4:F:2202:LEU:N	2.06	0.70
4:G:3201:LYS:HE3	4:G:3202:LEU:N	2.07	0.70
4:F:2131:ARG:HA	4:F:2131:ARG:NE	2.05	0.70
1:A:23:CYS:HB2	1:A:35:TRP:CH2	2.26	0.70
1:A:85:THR:OG1	1:A:103:LYS:HG2	1.92	0.70
1:A:89:GLN:HB2	1:A:98:PHE:CD1	2.27	0.70
1:A:41:ASP:OD1	1:A:43:THR:HG23	1.91	0.69
4:G:3034:CYS:HB2	4:G:3088:LEU:HD22	1.74	0.69
4:G:3038:ALA:HB1	4:G:3114:ILE:O	1.92	0.69
2:D:1559:SER:HA	4:G:3050:ASN:HD21	1.56	0.69
2:B:602:TRP:H	2:B:602:TRP:CD1	2.11	0.69
2:D:1516:VAL:HG12	2:D:1517:SER:H	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1528:THR:HB	2:D:1531:ASP:HB2	1.75	0.69
3:E:849:GLU:HG2	3:E:852:ARG:HH11	1.56	0.69
4:F:2034:CYS:HB2	4:F:2088:LEU:HD22	1.75	0.69
4:F:2038:ALA:HB1	4:F:2114:ILE:O	1.93	0.69
2:B:516:VAL:HG12	2:B:517:SER:H	1.56	0.68
1:C:1034:ASN:ND2	1:C:1089:GLN:HE22	1.88	0.68
4:F:2053:ILE:O	4:F:2053:ILE:HG12	1.94	0.68
1:A:34:ASN:ND2	1:A:89:GLN:HE22	1.88	0.68
2:D:1628:PRO:HG3	2:D:1713:LYS:HG2	1.76	0.68
2:D:1688:VAL:HG12	2:D:1689:THR:H	1.58	0.68
4:F:2135:VAL:HG22	4:F:2140:ALA:HA	1.74	0.68
4:G:3135:VAL:HG22	4:G:3140:ALA:HA	1.75	0.68
4:F:2042:PRO:HG2	4:F:2045:LEU:HB2	1.76	0.68
2:B:624:PRO:CB	2:B:650:TYR:HB3	2.18	0.67
2:B:528:THR:HB	2:B:531:ASP:HB2	1.76	0.67
3:E:829:PHE:CZ	3:E:857:LEU:HD13	2.29	0.67
1:C:1011:LEU:HD21	1:C:1019:VAL:HG12	1.77	0.67
1:C:1108:ARG:HG2	1:C:1171:SER:HB2	1.77	0.67
1:A:7:THR:HG21	3:E:849:GLU:OE1	1.94	0.67
2:D:1599:SER:HB2	2:D:1601:THR:O	1.95	0.67
4:G:3042:PRO:HG2	4:G:3045:LEU:HB2	1.77	0.67
1:A:108:ARG:HG2	1:A:171:SER:HB2	1.75	0.67
2:B:551:ILE:HD13	2:B:558:ALA:HB2	1.77	0.67
1:A:205:ILE:HD13	1:A:205:ILE:N	2.11	0.66
1:C:1091:GLY:CA	2:D:1603:TYR:HB2	2.26	0.66
1:A:11:LEU:HD21	1:A:19:VAL:HG12	1.77	0.66
4:G:3087:SER:O	4:G:3088:LEU:HG	1.96	0.66
4:G:3233:VAL:C	4:G:3234:ILE:HD12	2.21	0.66
2:D:1602:TRP:H	2:D:1602:TRP:CD1	2.13	0.66
1:C:1041:ASP:OD1	1:C:1043:THR:HG23	1.94	0.66
1:C:1006:GLN:CD	1:C:1100:GLY:H	2.03	0.66
4:F:2087:SER:O	4:F:2088:LEU:HG	1.96	0.65
4:G:3053:ILE:O	4:G:3053:ILE:HG12	1.96	0.65
2:B:599:SER:HB2	2:B:601:THR:O	1.95	0.65
2:B:506:GLN:N	2:B:610:GLN:OE1	2.21	0.65
4:F:2233:VAL:C	4:F:2234:ILE:HD12	2.21	0.65
4:G:3015:LYS:HA	4:G:3120:GLN:HG3	1.78	0.65
4:F:2038:ALA:HB2	4:F:2115:LYS:HB2	1.78	0.65
1:A:6:GLN:CD	1:A:100:GLY:H	2.04	0.65
4:F:2015:LYS:HA	4:F:2120:GLN:HG3	1.79	0.65
4:F:2180:GLN:HA	4:F:2194:SER:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2163:MET:O	4:F:2218:THR:HG23	1.97	0.65
1:C:1205:ILE:HD13	1:C:1205:ILE:N	2.10	0.65
2:D:1549:GLY:CA	2:D:1570:MET:HE1	2.26	0.65
4:G:3241:SER:HA	4:G:3243:GLU:N	2.13	0.64
4:F:2018:THR:HG22	4:F:2019:ALA:H	1.60	0.64
2:B:598:ARG:O	2:B:606:ASP:HB2	1.96	0.64
2:B:572:VAL:HG22	2:B:573:ASP:N	2.10	0.64
1:A:62:PHE:HD2	1:A:73:LEU:HD11	1.63	0.64
1:C:1121:SER:OG	2:D:1627:TYR:HB3	1.98	0.64
1:C:1193:THR:HG23	1:C:1208:SER:HB3	1.79	0.64
4:G:3163:MET:HE3	4:G:3251:LEU:HD21	1.79	0.64
1:C:1035:TRP:CZ3	1:C:1088:CYS:HB3	2.32	0.64
2:D:1518:VAL:CG1	2:D:1586:LEU:HD11	2.28	0.64
4:G:3163:MET:O	4:G:3218:THR:HG23	1.98	0.64
1:A:28:ASP:HA	1:A:68:GLY:O	1.98	0.64
1:C:1028:ASP:HA	1:C:1068:GLY:O	1.98	0.64
1:A:91:GLY:CA	2:B:603:TYR:HB2	2.27	0.64
4:F:2241:SER:HA	4:F:2243:GLU:N	2.13	0.64
4:G:3038:ALA:HB2	4:G:3115:LYS:HB2	1.79	0.63
2:B:561:ASN:O	2:B:562:GLN:C	2.42	0.63
4:F:2154:LYS:C	4:F:2155:LEU:HD22	2.23	0.63
4:G:3025:PRO:CA	4:G:3099:ILE:HD12	2.29	0.63
2:D:1506:GLN:N	2:D:1610:GLN:OE1	2.23	0.63
1:A:66:GLY:HA3	1:A:71:TYR:HA	1.81	0.63
2:D:1602:TRP:CZ2	4:G:3063:THR:HA	2.34	0.63
2:D:1657:LEU:HD22	2:D:1702:VAL:HG22	1.79	0.63
4:G:3018:THR:HG22	4:G:3019:ALA:H	1.62	0.63
2:D:1657:LEU:C	2:D:1657:LEU:HD13	2.24	0.62
4:F:2163:MET:HE3	4:F:2251:LEU:HD21	1.80	0.62
4:G:3180:GLN:HA	4:G:3194:SER:HA	1.80	0.62
2:D:1561:ASN:O	2:D:1562:GLN:C	2.42	0.62
2:D:1528:THR:HG22	2:D:1531:ASP:H	1.65	0.62
2:B:628:PRO:HG3	2:B:713:LYS:HG2	1.81	0.62
4:G:3023:LEU:O	4:G:3129:GLN:HG3	2.00	0.62
2:B:549:GLY:CA	2:B:570:MET:HE1	2.28	0.62
1:C:1066:GLY:HA3	1:C:1071:TYR:HA	1.82	0.62
3:E:842:THR:CG2	3:E:845:GLU:H	2.13	0.62
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.82	0.62
4:F:2025:PRO:CA	4:F:2099:ILE:HD12	2.30	0.61
4:G:3080:TRP:HB3	4:G:3096:THR:O	2.00	0.61
1:A:13:ALA:HA	3:E:835:GLN:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HD3	1:A:109:ALA:O	2.00	0.61
2:B:602:TRP:CZ2	4:F:2063:THR:HA	2.35	0.61
4:F:2023:LEU:O	4:F:2129:GLN:HG3	2.00	0.61
2:B:636:THR:C	2:B:638:GLY:H	2.08	0.61
1:C:1037:GLN:HB2	1:C:1047:LEU:HD11	1.81	0.61
2:D:1507:SER:O	2:D:1612:THR:HG23	2.00	0.61
2:D:1598:ARG:O	2:D:1606:ASP:HB2	2.00	0.61
4:F:2030:PHE:CD1	4:F:2095:LEU:HB3	2.36	0.61
2:B:657:LEU:HD22	2:B:702:VAL:HG22	1.81	0.61
2:D:1682:LEU:HD23	2:D:1682:LEU:C	2.25	0.61
3:E:842:THR:HG22	3:E:845:GLU:HB2	1.82	0.61
2:B:657:LEU:C	2:B:657:LEU:HD13	2.25	0.61
4:G:3131:ARG:HA	4:G:3131:ARG:HE	1.66	0.61
2:D:1501:GLN:OE1	2:D:1501:GLN:N	2.34	0.61
2:D:1551:ILE:HD13	2:D:1558:ALA:HB2	1.82	0.61
4:F:2172:VAL:O	4:F:2237:CYS:HB3	2.00	0.61
2:B:507:SER:O	2:B:612:THR:HG23	2.01	0.61
4:G:3193:LYS:O	4:G:3194:SER:HB2	1.99	0.61
4:G:3233:VAL:HG22	4:G:3253:PHE:HE1	1.66	0.60
2:B:501:GLN:OE1	2:B:501:GLN:N	2.34	0.60
2:B:518:VAL:CG1	2:B:586:LEU:HD11	2.31	0.60
1:C:1036:TYR:CD2	1:C:1046:LEU:HD23	2.36	0.60
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.36	0.60
1:A:205:ILE:H	1:A:205:ILE:CD1	2.05	0.60
2:B:682:LEU:HD23	2:B:682:LEU:C	2.26	0.60
4:F:2080:TRP:CZ3	4:F:2097:VAL:HG13	2.37	0.60
4:F:2193:LYS:O	4:F:2194:SER:HB2	1.99	0.60
4:G:3080:TRP:CZ3	4:G:3097:VAL:HG13	2.36	0.60
1:A:122:SER:HA	1:A:125:LEU:HD12	1.83	0.60
1:A:136:LEU:HD12	1:A:136:LEU:N	2.17	0.59
4:G:3030:PHE:CD1	4:G:3095:LEU:HB3	2.36	0.59
1:A:11:LEU:O	1:A:11:LEU:HG	2.02	0.59
1:A:36:TYR:CD2	1:A:46:LEU:HD23	2.38	0.59
2:B:692:THR:HG22	2:B:692:THR:O	2.02	0.59
4:F:2131:ARG:HA	4:F:2131:ARG:HE	1.66	0.59
4:G:3230:SER:C	4:G:3231:LYS:HD2	2.28	0.59
2:D:1628:PRO:HG3	2:D:1713:LYS:CG	2.33	0.59
4:F:2233:VAL:HG22	4:F:2253:PHE:HE1	1.65	0.59
1:C:1002:ILE:HD11	1:C:1029:ILE:CG2	2.32	0.59
2:D:1675:LEU:HD23	2:D:1680:TYR:CD1	2.37	0.59
4:G:3172:VAL:O	4:G:3237:CYS:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1516:VAL:CG1	2:D:1517:SER:N	2.66	0.59
4:G:3175:PRO:HG2	4:G:3181:TYR:HA	1.85	0.59
1:C:1023:CYS:SG	1:C:1033:LEU:HD11	2.43	0.58
4:G:3030:PHE:HD1	4:G:3095:LEU:HB3	1.67	0.58
4:F:2080:TRP:HB3	4:F:2096:THR:O	2.03	0.58
2:D:1624:PRO:HB3	2:D:1650:TYR:CB	2.24	0.58
3:E:845:GLU:HB3	3:E:849:GLU:OE1	2.03	0.58
4:F:2175:PRO:HG2	4:F:2181:TYR:HA	1.85	0.58
2:B:604:TYR:C	2:B:604:TYR:CD2	2.82	0.58
3:E:864:TYR:HB2	3:E:878:LYS:O	2.04	0.58
2:D:1604:TYR:C	2:D:1604:TYR:CD2	2.81	0.58
2:B:693:TRP:CD1	2:B:694:PRO:HA	2.37	0.58
1:C:1205:ILE:H	1:C:1205:ILE:CD1	2.04	0.58
4:F:2030:PHE:HD1	4:F:2095:LEU:HB3	1.68	0.58
4:G:3018:THR:HG22	4:G:3019:ALA:N	2.19	0.58
4:G:3141:ARG:HG2	4:G:3166:VAL:HB	1.85	0.58
4:G:3154:LYS:C	4:G:3155:LEU:HD22	2.29	0.58
4:G:3180:GLN:HG2	4:G:3193:LYS:O	2.03	0.58
2:B:688:VAL:HG11	2:B:692:THR:HG21	1.85	0.57
1:C:1122:SER:HA	1:C:1125:LEU:HD12	1.85	0.57
1:C:1026:SER:O	1:C:1027:GLN:CB	2.51	0.57
1:C:1188:ARG:O	1:C:1189:HIS:ND1	2.37	0.57
2:D:1692:THR:HG22	2:D:1692:THR:O	2.04	0.57
4:F:2018:THR:HG22	4:F:2019:ALA:N	2.18	0.57
4:F:2180:GLN:HG2	4:F:2193:LYS:O	2.03	0.57
4:F:2230:SER:C	4:F:2231:LYS:HD2	2.29	0.57
1:A:2:ILE:HD11	1:A:29:ILE:CG2	2.34	0.57
2:B:692:THR:O	2:B:692:THR:CG2	2.51	0.57
1:C:1086:TYR:O	1:C:1101:GLY:HA2	2.04	0.57
2:D:1536:TRP:CE3	2:D:1581:MET:HG3	2.40	0.57
2:D:1692:THR:O	2:D:1692:THR:CG2	2.53	0.57
4:F:2178:ASN:HB3	4:F:2207:TRP:CD1	2.39	0.57
2:B:536:TRP:CE3	2:B:581:MET:HG3	2.39	0.57
3:E:858:ALA:O	3:E:860:VAL:N	2.37	0.57
4:G:3178:ASN:HB3	4:G:3207:TRP:CD1	2.40	0.57
4:G:3199:LEU:HD11	4:G:3227:PRO:CD	2.33	0.57
1:C:1089:GLN:HB2	1:C:1098:PHE:CE1	2.40	0.57
3:E:876:ASN:C	3:E:877:ILE:HG13	2.29	0.57
4:F:2062:CYS:SG	4:F:2062:CYS:O	2.62	0.57
2:D:1604:TYR:C	2:D:1604:TYR:HD2	2.13	0.57
1:A:6:GLN:CD	1:A:101:GLY:H	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:NE2	1:A:101:GLY:H	2.03	0.57
1:A:26:SER:O	1:A:27:GLN:CB	2.52	0.57
1:A:137:ASN:HA	1:A:174:SER:OG	2.05	0.57
2:D:1636:THR:O	2:D:1638:GLY:N	2.31	0.57
4:F:2122:CYS:C	4:F:2123:MET:HE2	2.30	0.57
1:C:1108:ARG:HD3	1:C:1109:ALA:O	2.05	0.56
4:F:2183:SER:CB	4:F:2191:ASN:HD22	2.14	0.56
1:A:135:PHE:C	1:A:136:LEU:HD12	2.30	0.56
2:B:528:THR:HG22	2:B:531:ASP:H	1.69	0.56
2:D:1636:THR:C	2:D:1638:GLY:H	2.10	0.56
1:A:31:ASN:HA	1:A:51:THR:OG1	2.05	0.56
2:B:535:HIS:O	2:B:596:CYS:HA	2.06	0.56
1:C:1055:HIS:O	1:C:1058:VAL:HG23	2.06	0.56
2:D:1516:VAL:CG1	2:D:1517:SER:H	2.19	0.56
1:C:1137:ASN:HA	1:C:1174:SER:OG	2.06	0.56
4:G:3062:CYS:O	4:G:3062:CYS:SG	2.63	0.56
4:G:3082:THR:HG22	4:G:3082:THR:O	2.04	0.56
1:C:1210:ASN:O	1:C:1212:ASN:N	2.39	0.56
4:G:3034:CYS:H	4:G:3088:LEU:HD22	1.69	0.56
1:C:1004:VAL:HA	1:C:1025:ALA:HA	1.88	0.56
4:F:2082:THR:HG22	4:F:2082:THR:O	2.05	0.56
1:C:1006:GLN:NE2	1:C:1101:GLY:H	2.03	0.56
1:C:1047:LEU:CD1	1:C:1086:TYR:HE2	2.18	0.56
2:D:1572:VAL:HG22	2:D:1573:ASP:N	2.12	0.56
4:G:3070:SER:C	4:G:3072:LEU:H	2.14	0.56
4:G:3081:TRP:HA	4:G:3094:LYS:O	2.06	0.56
2:B:591:SER:O	2:B:592:ALA:HB2	2.06	0.56
2:B:636:THR:O	2:B:638:GLY:N	2.31	0.55
2:B:506:GLN:HE22	2:B:595:TYR:HA	1.71	0.55
2:B:624:PRO:HB3	2:B:650:TYR:CB	2.25	0.55
1:C:1062:PHE:HD2	1:C:1073:LEU:HD11	1.70	0.55
1:C:1118:PHE:HE1	1:C:1135:PHE:HD2	1.54	0.55
1:C:1014:SER:O	1:C:1015:LEU:C	2.49	0.55
2:D:1693:TRP:CD1	2:D:1694:PRO:HA	2.41	0.55
4:F:2034:CYS:H	4:F:2088:LEU:HD22	1.71	0.55
4:F:2066:ALA:O	4:F:2067:VAL:HG13	2.07	0.55
4:F:2112:GLY:HA3	4:F:2123:MET:CE	2.36	0.55
4:G:3017:SER:O	4:G:3122:CYS:HA	2.06	0.55
1:C:1032:TYR:OH	4:G:3038:ALA:HA	2.06	0.55
4:G:3034:CYS:H	4:G:3088:LEU:CD2	2.20	0.55
4:G:3109:PHE:CD1	4:G:3109:PHE:C	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:OG	2:B:627:TYR:HB3	2.05	0.55
2:B:516:VAL:CG1	2:B:517:SER:H	2.19	0.55
2:B:628:PRO:HG3	2:B:713:LYS:CG	2.36	0.55
2:D:1535:HIS:O	2:D:1596:CYS:HA	2.06	0.55
4:G:3122:CYS:C	4:G:3123:MET:HE2	2.32	0.55
1:C:1113:PRO:CA	1:C:1139:PHE:HB3	2.37	0.55
2:D:1504:LEU:HD22	2:D:1524:GLY:HA2	1.88	0.55
4:F:2199:LEU:HD11	4:F:2227:PRO:CD	2.34	0.55
1:A:133:VAL:HG12	1:A:134:CYS:N	2.22	0.55
1:C:1093:THR:HA	4:G:3047:TYR:OH	2.07	0.55
2:D:1591:SER:O	2:D:1592:ALA:HB2	2.07	0.55
4:F:2172:VAL:HG12	4:F:2173:LYS:N	2.22	0.55
1:A:209:PHE:HB2	2:B:632:VAL:HG11	1.88	0.54
2:B:516:VAL:CG1	2:B:517:SER:N	2.67	0.54
4:G:3172:VAL:HG12	4:G:3173:LYS:N	2.22	0.54
1:C:1006:GLN:CD	1:C:1101:GLY:H	2.16	0.54
4:F:2017:SER:O	4:F:2122:CYS:HA	2.08	0.54
4:F:2055:PRO:HG2	4:F:2058:THR:CG2	2.37	0.54
1:C:1003:GLN:HG3	1:C:1003:GLN:O	2.08	0.54
2:D:1675:LEU:HD23	2:D:1680:TYR:CE1	2.42	0.54
4:G:3228:ALA:HB3	4:G:3229:GLU:OE1	2.07	0.54
2:B:504:LEU:HD22	2:B:524:GLY:HA2	1.89	0.54
2:B:530:THR:HG22	2:B:554:TYR:HB2	1.88	0.54
2:B:604:TYR:C	2:B:604:TYR:HD2	2.14	0.54
2:B:628:PRO:O	2:B:629:LEU:HD23	2.07	0.54
1:C:1011:LEU:HG	1:C:1011:LEU:O	2.06	0.54
4:G:3042:PRO:O	4:G:3043:PRO:C	2.50	0.54
4:G:3112:GLY:HA3	4:G:3123:MET:CE	2.37	0.54
1:A:50:TYR:O	1:A:52:SER:N	2.37	0.54
1:C:1031:ASN:HA	1:C:1051:THR:OG1	2.07	0.54
1:A:89:GLN:HB2	1:A:98:PHE:CE1	2.41	0.54
1:A:86:TYR:O	1:A:101:GLY:HA2	2.07	0.54
4:G:3053:ILE:HD13	4:G:3067:VAL:O	2.08	0.54
1:A:4:VAL:HG23	1:A:99:GLY:HA2	1.89	0.54
2:D:1512:VAL:HG12	2:D:1513:ARG:N	2.23	0.54
2:D:1675:LEU:HD13	2:D:1676:GLN:N	2.22	0.54
2:B:547:TRP:CH2	2:B:549:GLY:HA2	2.43	0.53
2:D:1688:VAL:HG11	2:D:1692:THR:HG21	1.90	0.53
4:F:2059:THR:O	4:F:2060:SER:HB3	2.07	0.53
4:F:2210:ASN:O	4:F:2211:ALA:C	2.51	0.53
4:G:3055:PRO:HG2	4:G:3058:THR:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:SER:O	1:A:15:LEU:C	2.51	0.53
1:A:113:PRO:CA	1:A:139:PHE:HB3	2.38	0.53
1:A:188:ARG:O	1:A:189:HIS:ND1	2.41	0.53
1:C:1038:GLN:HG3	1:C:1044:VAL:HG22	1.88	0.53
2:D:1506:GLN:HE22	2:D:1595:TYR:HA	1.73	0.53
4:F:2034:CYS:H	4:F:2088:LEU:CD2	2.21	0.53
4:F:2044:THR:HG21	4:F:2052:GLN:OE1	2.08	0.53
4:G:3103:PRO:HG2	4:G:3105:THR:O	2.09	0.53
1:A:170:ASP:OD1	1:A:170:ASP:C	2.52	0.53
1:C:1004:VAL:HG23	1:C:1099:GLY:HA2	1.91	0.53
4:F:2070:SER:C	4:F:2072:LEU:H	2.15	0.53
4:F:2099:ILE:HA	4:F:2102:PHE:CE1	2.43	0.53
4:F:2109:PHE:CD1	4:F:2109:PHE:C	2.87	0.53
4:F:2216:GLY:O	4:F:2217:ALA:HB2	2.08	0.53
2:B:688:VAL:HG12	2:B:689:THR:N	2.23	0.53
1:C:1089:GLN:OE1	2:D:1603:TYR:O	2.26	0.53
1:C:1135:PHE:C	1:C:1136:LEU:HD12	2.33	0.53
1:A:55:HIS:O	1:A:58:VAL:HG23	2.08	0.53
4:F:2103:PRO:HG2	4:F:2105:THR:O	2.09	0.53
4:G:3059:THR:O	4:G:3060:SER:HB3	2.08	0.53
4:G:3216:GLY:O	4:G:3217:ALA:HB2	2.08	0.53
1:A:4:VAL:HA	1:A:25:ALA:HA	1.89	0.53
1:A:37:GLN:HB2	1:A:47:LEU:CD1	2.39	0.53
4:F:2038:ALA:HB2	4:F:2115:LYS:CB	2.38	0.53
4:F:2042:PRO:O	4:F:2043:PRO:C	2.51	0.53
4:F:2241:SER:HA	4:F:2243:GLU:H	1.73	0.53
4:G:3050:ASN:O	4:G:3051:ARG:C	2.51	0.53
1:A:62:PHE:CD2	1:A:73:LEU:HD11	2.44	0.53
1:C:1050:TYR:O	1:C:1052:SER:N	2.37	0.53
1:A:210:ASN:O	1:A:212:ASN:N	2.41	0.53
2:B:561:ASN:OD1	2:B:563:LYS:HD3	2.09	0.53
1:C:1062:PHE:CE2	1:C:1075:ILE:HG12	2.43	0.53
2:B:675:LEU:HD13	2:B:676:GLN:N	2.23	0.52
4:F:2228:ALA:HB3	4:F:2229:GLU:OE1	2.09	0.52
2:D:1657:LEU:C	2:D:1657:LEU:CD1	2.83	0.52
4:G:3025:PRO:HA	4:G:3099:ILE:CD1	2.38	0.52
1:A:39:LYS:HB3	1:A:40:PRO:HD2	1.91	0.52
2:D:1549:GLY:C	2:D:1570:MET:HE1	2.35	0.52
2:D:1670:THR:HA	2:D:1684:SER:HA	1.92	0.52
4:G:3210:ASN:O	4:G:3211:ALA:C	2.52	0.52
4:F:2081:TRP:HA	4:F:2094:LYS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3046:ALA:O	4:G:3084:ASP:HA	2.10	0.52
2:B:512:VAL:HG12	2:B:513:ARG:N	2.23	0.52
1:C:1007:THR:OG1	3:E:855:ASP:OD1	2.28	0.52
1:C:1133:VAL:HG12	1:C:1134:CYS:N	2.24	0.52
2:D:1704:HIS:NE2	2:D:1706:ALA:HB3	2.24	0.52
4:F:2203:THR:O	4:F:2205:ASN:N	2.43	0.52
4:G:3203:THR:O	4:G:3205:ASN:N	2.43	0.52
1:A:3:GLN:O	1:A:3:GLN:HG3	2.09	0.52
3:E:853:TYR:HE1	3:E:857:LEU:HD11	1.75	0.52
1:A:32:TYR:OH	4:F:2038:ALA:HA	2.08	0.52
1:A:193:THR:CG2	1:A:208:SER:HB3	2.39	0.52
2:B:559:SER:HA	4:F:2050:ASN:ND2	2.24	0.52
2:B:632:VAL:O	2:B:634:GLY:N	2.43	0.52
4:G:3198:ILE:O	4:G:3199:LEU:HD22	2.10	0.52
1:A:47:LEU:CD1	1:A:86:TYR:HE2	2.23	0.52
2:D:1530:THR:HG22	2:D:1554:TYR:HB2	1.91	0.52
1:C:1209:PHE:HB2	2:D:1632:VAL:HG11	1.91	0.52
2:D:1561:ASN:OD1	2:D:1563:LYS:HD3	2.10	0.52
4:F:2046:ALA:O	4:F:2084:ASP:HA	2.09	0.52
4:G:3099:ILE:HA	4:G:3102:PHE:CE1	2.45	0.52
4:G:3241:SER:HA	4:G:3243:GLU:H	1.72	0.52
1:A:46:LEU:HD13	1:A:46:LEU:O	2.10	0.52
2:B:657:LEU:C	2:B:657:LEU:CD1	2.83	0.52
2:B:670:THR:HA	2:B:684:SER:HA	1.92	0.52
3:E:868:LEU:O	3:E:869:GLU:HG2	2.10	0.52
4:G:3038:ALA:HB2	4:G:3115:LYS:CB	2.39	0.52
3:E:842:THR:HG23	3:E:844:GLU:H	1.75	0.51
1:A:38:GLN:HG3	1:A:44:VAL:HG22	1.92	0.51
1:A:89:GLN:OE1	2:B:603:TYR:O	2.28	0.51
4:G:3199:LEU:HD21	4:G:3227:PRO:HD3	1.93	0.51
1:A:9:SER:CB	3:E:840:LYS:HE2	2.41	0.51
3:E:845:GLU:C	3:E:847:THR:N	2.68	0.51
4:F:2221:ILE:O	4:F:2222:LYS:C	2.54	0.51
1:C:1037:GLN:HB2	1:C:1047:LEU:CD1	2.40	0.51
1:C:1124:GLN:O	1:C:1124:GLN:HG2	2.09	0.51
2:D:1547:TRP:CH2	2:D:1549:GLY:HA2	2.45	0.51
4:F:2024:THR:HB	4:F:2025:PRO:HD2	1.91	0.51
2:B:530:THR:HG21	2:B:554:TYR:HD1	1.75	0.51
1:C:1065:SER:O	1:C:1072:SER:N	2.41	0.51
1:C:1108:ARG:HH12	1:C:1111:ALA:HB2	1.75	0.51
4:F:2113:CYS:HB2	4:F:2122:CYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:633:CYS:SG	2:B:634:GLY:N	2.84	0.51
4:F:2201:LYS:O	4:F:2225:ALA:HB1	2.11	0.51
4:G:3044:THR:HG21	4:G:3052:GLN:OE1	2.10	0.51
4:F:2141:ARG:HG2	4:F:2166:VAL:HB	1.92	0.51
1:A:65:SER:O	1:A:72:SER:N	2.42	0.51
4:G:3076:ALA:HA	4:G:3080:TRP:CH2	2.46	0.51
2:B:540:SER:O	2:B:544:SER:N	2.44	0.50
4:F:2155:LEU:O	4:F:2226:PHE:HE2	1.94	0.50
4:G:3201:LYS:O	4:G:3225:ALA:HB1	2.10	0.50
4:F:2053:ILE:HD13	4:F:2067:VAL:O	2.12	0.50
4:F:2161:THR:O	4:F:2162:THR:HB	2.11	0.50
4:G:3087:SER:HB3	4:G:3092:GLY:H	1.77	0.50
4:G:3183:SER:CB	4:G:3191:ASN:HD22	2.14	0.50
4:G:3025:PRO:HB3	4:G:3099:ILE:HG23	1.93	0.50
2:B:603:TYR:CD2	2:B:604:TYR:N	2.79	0.50
3:E:845:GLU:C	3:E:847:THR:H	2.18	0.50
4:F:2025:PRO:HB3	4:F:2099:ILE:HG23	1.93	0.50
4:G:3045:LEU:HD11	4:G:3081:TRP:CZ3	2.47	0.50
2:B:660:ASN:ND2	2:B:699:THR:H	2.10	0.50
2:B:551:ILE:HD12	2:B:557:ASP:O	2.12	0.50
2:D:1530:THR:HG21	2:D:1554:TYR:HD1	1.76	0.50
4:F:2112:GLY:HA3	4:F:2123:MET:SD	2.52	0.50
4:G:3066:ALA:O	4:G:3067:VAL:HG13	2.11	0.50
4:G:3221:ILE:O	4:G:3222:LYS:C	2.54	0.50
2:D:1573:ASP:O	2:D:1574:LYS:C	2.54	0.50
4:F:2174:VAL:HG13	4:F:2175:PRO:HA	1.93	0.50
1:A:93:THR:HA	4:F:2047:TYR:OH	2.11	0.50
2:D:1605:PHE:N	2:D:1605:PHE:CD2	2.79	0.50
2:D:1688:VAL:HG12	2:D:1689:THR:N	2.27	0.50
4:F:2045:LEU:HD11	4:F:2081:TRP:CZ3	2.47	0.50
4:F:2209:GLY:O	4:F:2211:ALA:N	2.44	0.50
1:A:34:ASN:ND2	1:A:89:GLN:NE2	2.44	0.49
1:C:1170:ASP:OD1	1:C:1170:ASP:C	2.54	0.49
2:D:1603:TYR:CD2	2:D:1604:TYR:N	2.80	0.49
3:E:876:ASN:N	3:E:876:ASN:HD22	2.10	0.49
4:F:2025:PRO:HA	4:F:2099:ILE:CD1	2.39	0.49
1:C:1083:ILE:HG23	1:C:1104:LEU:O	2.13	0.49
1:C:1113:PRO:HA	1:C:1139:PHE:HB3	1.94	0.49
2:D:1636:THR:C	2:D:1638:GLY:N	2.70	0.49
3:E:844:GLU:N	3:E:844:GLU:CD	2.70	0.49
3:E:853:TYR:CE1	3:E:857:LEU:HD11	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2050:ASN:O	4:F:2051:ARG:C	2.54	0.49
4:G:3253:PHE:N	4:G:3253:PHE:CD1	2.80	0.49
1:A:62:PHE:CE2	1:A:75:ILE:HG12	2.47	0.49
1:C:1002:ILE:O	1:C:1002:ILE:CG1	2.42	0.49
1:C:1210:ASN:O	1:C:1211:ARG:C	2.55	0.49
4:F:2253:PHE:CD1	4:F:2253:PHE:N	2.79	0.49
1:C:1046:LEU:HD13	1:C:1046:LEU:O	2.13	0.49
1:C:1190:ASN:OD1	1:C:1210:ASN:HB3	2.13	0.49
4:F:2199:LEU:HD21	4:F:2227:PRO:HD3	1.94	0.49
4:G:3113:CYS:HB2	4:G:3122:CYS:HB3	1.95	0.49
2:D:1549:GLY:HA3	2:D:1570:MET:CE	2.36	0.49
4:F:2087:SER:HB3	4:F:2092:GLY:H	1.77	0.49
1:A:150:ILE:HG22	1:A:189:HIS:CD2	2.48	0.49
4:G:3108:THR:CG2	4:G:3127:THR:HG23	2.42	0.49
4:G:3209:GLY:O	4:G:3211:ALA:N	2.45	0.49
1:C:1096:TYR:CZ	2:D:1603:TYR:HA	2.48	0.49
3:E:824:LYS:C	3:E:825:VAL:HG23	2.38	0.49
4:G:3157:ALA:HB2	4:G:3226:PHE:CD2	2.48	0.49
4:G:3184:GLY:H	4:G:3191:ASN:HB3	1.77	0.49
2:B:591:SER:HA	2:B:614:LEU:O	2.13	0.49
2:B:602:TRP:CG	4:F:2063:THR:HG22	2.48	0.49
1:C:1011:LEU:HA	3:E:866:ALA:O	2.13	0.49
1:C:1136:LEU:HD12	1:C:1136:LEU:N	2.27	0.49
2:D:1602:TRP:CD2	4:G:3063:THR:HG22	2.48	0.49
3:E:829:PHE:HB2	3:E:833:LYS:O	2.12	0.49
4:F:2115:LYS:O	4:F:2117:ASP:N	2.41	0.49
1:A:118:PHE:HE1	1:A:135:PHE:HD2	1.59	0.49
2:B:522:CYS:HB2	2:B:536:TRP:CH2	2.48	0.49
2:B:675:LEU:HD23	2:B:680:TYR:CD1	2.47	0.49
3:E:869:GLU:O	3:E:871:GLY:N	2.46	0.49
4:G:3115:LYS:O	4:G:3117:ASP:N	2.42	0.49
1:A:23:CYS:SG	1:A:33:LEU:HD11	2.53	0.48
2:B:549:GLY:HA3	2:B:570:MET:CE	2.39	0.48
2:B:605:PHE:CD2	2:B:605:PHE:N	2.79	0.48
1:C:1150:ILE:HG22	1:C:1189:HIS:CD2	2.48	0.48
4:F:2076:ALA:HA	4:F:2080:TRP:CH2	2.48	0.48
4:F:2184:GLY:H	4:F:2191:ASN:HB3	1.77	0.48
1:A:190:ASN:OD1	1:A:210:ASN:HB3	2.13	0.48
4:G:3024:THR:HB	4:G:3025:PRO:HD2	1.93	0.48
1:A:200:THR:O	1:A:201:SER:HB2	2.12	0.48
1:C:1023:CYS:HB2	1:C:1035:TRP:HH2	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1538:LYS:NZ	2:D:1590:ASP:HA	2.28	0.48
1:A:151:ASP:HA	1:A:191:SER:HB2	1.95	0.48
2:B:549:GLY:C	2:B:570:MET:HE1	2.38	0.48
1:C:1154:GLU:HG2	1:C:1155:ARG:H	1.77	0.48
1:A:133:VAL:CG1	1:A:134:CYS:N	2.76	0.48
1:A:210:ASN:O	1:A:211:ARG:C	2.56	0.48
2:B:553:THR:OG1	4:F:2064:SER:HB2	2.14	0.48
2:B:573:ASP:O	2:B:574:LYS:C	2.56	0.48
2:D:1694:PRO:O	2:D:1695:SER:C	2.56	0.48
4:F:2110:VAL:HG12	4:F:2111:VAL:N	2.28	0.48
1:A:113:PRO:HA	1:A:139:PHE:HB3	1.95	0.48
1:C:1200:THR:O	1:C:1201:SER:HB2	2.13	0.48
4:F:2041:GLU:HG3	4:F:2042:PRO:HD3	1.96	0.48
2:B:602:TRP:CD2	4:F:2063:THR:HG22	2.49	0.48
1:C:1154:GLU:HG2	1:C:1155:ARG:N	2.29	0.48
1:C:1195:GLU:HG3	1:C:1206:VAL:HG13	1.95	0.48
4:F:2198:ILE:O	4:F:2199:LEU:HD22	2.13	0.48
1:C:1039:LYS:HB3	1:C:1040:PRO:HD2	1.95	0.48
4:G:3174:VAL:HG13	4:G:3175:PRO:HA	1.95	0.48
1:C:1151:ASP:HA	1:C:1191:SER:HB2	1.96	0.48
2:D:1540:SER:O	2:D:1544:SER:N	2.47	0.48
1:A:23:CYS:HB2	1:A:35:TRP:HH2	1.77	0.48
1:C:1013:ALA:O	1:C:1107:LYS:N	2.45	0.48
1:C:1006:GLN:OE1	1:C:1099:GLY:HA3	2.14	0.47
2:D:1633:CYS:SG	2:D:1634:GLY:N	2.87	0.47
4:G:3102:PHE:HB3	4:G:3103:PRO:HD2	1.96	0.47
2:B:694:PRO:O	2:B:695:SER:C	2.56	0.47
1:C:1118:PHE:CE1	1:C:1135:PHE:HD2	2.30	0.47
1:C:1133:VAL:CG1	1:C:1134:CYS:N	2.77	0.47
1:C:1204:PRO:O	1:C:1206:VAL:HG23	2.14	0.47
2:D:1560:TYR:OH	2:D:1569:THR:HA	2.13	0.47
4:F:2108:THR:CG2	4:F:2127:THR:HG23	2.43	0.47
4:G:3112:GLY:HA3	4:G:3123:MET:HA	1.96	0.47
3:E:823:ILE:HD12	3:E:823:ILE:N	2.29	0.47
1:A:154:GLU:HG2	1:A:155:ARG:N	2.30	0.47
2:B:636:THR:C	2:B:638:GLY:N	2.70	0.47
1:C:1055:HIS:ND1	1:C:1055:HIS:C	2.72	0.47
2:D:1559:SER:HA	4:G:3050:ASN:ND2	2.27	0.47
2:B:602:TRP:CD1	2:B:602:TRP:N	2.80	0.47
1:C:1119:PRO:HB3	1:C:1209:PHE:CE1	2.49	0.47
2:D:1591:SER:HA	2:D:1614:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3041:GLU:HG3	4:G:3042:PRO:HD3	1.95	0.47
1:A:195:GLU:HG3	1:A:206:VAL:HG13	1.96	0.47
1:C:1092:ASN:OD1	4:G:3039:LEU:HD11	2.15	0.47
3:E:868:LEU:CD2	3:E:875:MET:HE2	2.45	0.47
4:F:2042:PRO:HG2	4:F:2045:LEU:CB	2.44	0.47
4:F:2141:ARG:HA	4:F:2166:VAL:HB	1.97	0.47
4:F:2174:VAL:HA	4:F:2175:PRO:C	2.40	0.47
4:G:3110:VAL:HG12	4:G:3111:VAL:N	2.28	0.47
4:G:3112:GLY:HA3	4:G:3123:MET:SD	2.55	0.47
1:A:83:ILE:HG23	1:A:104:LEU:O	2.15	0.47
2:B:587:THR:C	2:B:589:GLU:H	2.23	0.47
1:C:1047:LEU:HD11	1:C:1086:TYR:HE2	1.79	0.47
2:D:1551:ILE:HD12	2:D:1557:ASP:O	2.14	0.47
4:F:2201:LYS:HE3	4:F:2202:LEU:H	1.79	0.47
1:A:193:THR:OG1	1:A:208:SER:HB3	2.14	0.47
2:D:1517:SER:HB2	2:D:1584:ALA:HA	1.97	0.47
2:D:1657:LEU:HD23	2:D:1702:VAL:HG22	1.92	0.47
4:F:2178:ASN:HB3	4:F:2207:TRP:CG	2.50	0.47
1:C:1055:HIS:C	1:C:1055:HIS:HD1	2.23	0.47
1:C:1175:MET:CE	1:C:1177:SER:HB2	2.45	0.47
2:D:1602:TRP:CG	4:G:3063:THR:HG22	2.50	0.47
1:A:96:TYR:CZ	2:B:603:TYR:HA	2.50	0.46
1:A:108:ARG:HH12	1:A:111:ALA:HB2	1.80	0.46
2:D:1632:VAL:O	2:D:1634:GLY:N	2.48	0.46
4:F:2099:ILE:HA	4:F:2102:PHE:CD1	2.51	0.46
4:F:2253:PHE:H	4:F:2253:PHE:HD1	1.64	0.46
1:A:24:ARG:NH2	3:E:852:ARG:NH2	2.64	0.46
2:B:538:LYS:NZ	2:B:590:ASP:HA	2.30	0.46
2:D:1587:THR:C	2:D:1589:GLU:H	2.23	0.46
4:F:2047:TYR:C	4:F:2049:PRO:CD	2.88	0.46
1:A:55:HIS:C	1:A:55:HIS:ND1	2.73	0.46
4:F:2098:PRO:HB3	4:F:2100:GLU:OE1	2.15	0.46
1:C:1193:THR:OG1	1:C:1208:SER:HB3	2.16	0.46
4:G:3040:THR:HG21	4:G:3046:ALA:HB2	1.97	0.46
1:A:204:PRO:O	1:A:206:VAL:HG23	2.15	0.46
4:F:2106:THR:HG23	4:F:2128:VAL:O	2.15	0.46
1:C:1002:ILE:HD11	1:C:1029:ILE:HG22	1.97	0.46
1:C:1195:GLU:HG3	1:C:1206:VAL:HG22	1.98	0.46
1:A:124:GLN:O	1:A:124:GLN:HG2	2.15	0.46
1:A:154:GLU:HG2	1:A:155:ARG:H	1.80	0.46
2:B:632:VAL:O	2:B:633:CYS:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:651:PHE:C	2:B:651:PHE:CD2	2.93	0.46
2:B:675:LEU:HD23	2:B:680:TYR:CE1	2.50	0.46
1:C:1035:TRP:CE3	1:C:1088:CYS:HB3	2.50	0.46
4:G:3076:ALA:O	4:G:3077:GLU:HG2	2.15	0.46
4:G:3110:VAL:O	4:G:3111:VAL:HG13	2.16	0.46
2:B:603:TYR:CE2	2:B:604:TYR:CD1	3.04	0.46
2:B:675:LEU:HD13	2:B:675:LEU:C	2.41	0.46
4:G:3060:SER:OG	4:G:3061:SER:N	2.47	0.46
4:G:3174:VAL:HA	4:G:3175:PRO:C	2.41	0.46
1:A:2:ILE:HG21	1:A:93:THR:HB	1.97	0.46
1:C:1001:ASP:N	1:C:1095:PRO:HD2	2.30	0.46
2:D:1671:PHE:HB3	2:D:1672:PRO:HD2	1.97	0.46
4:F:2076:ALA:O	4:F:2077:GLU:HG2	2.16	0.46
4:G:3009:VAL:HG22	4:G:3031:THR:CB	2.42	0.46
4:G:3099:ILE:HA	4:G:3102:PHE:CD1	2.51	0.46
4:G:3161:THR:O	4:G:3162:THR:HB	2.15	0.46
2:B:671:PHE:HB3	2:B:672:PRO:HD2	1.98	0.46
1:C:1125:LEU:C	1:C:1127:SER:H	2.24	0.46
2:D:1628:PRO:O	2:D:1629:LEU:HD23	2.16	0.46
4:F:2102:PHE:HB3	4:F:2103:PRO:HD2	1.97	0.46
1:A:92:ASN:OD1	4:F:2039:LEU:HD11	2.16	0.45
4:G:3042:PRO:HG2	4:G:3045:LEU:CB	2.45	0.45
4:G:3233:VAL:HG22	4:G:3251:LEU:HB2	1.97	0.45
2:B:631:PRO:O	2:B:718:ARG:HD2	2.17	0.45
4:G:3178:ASN:HB3	4:G:3207:TRP:CG	2.50	0.45
1:A:121:SER:C	1:A:123:GLU:N	2.74	0.45
2:B:539:GLN:HB2	2:B:545:LEU:CD2	2.47	0.45
2:B:602:TRP:CD1	4:F:2063:THR:HG22	2.51	0.45
2:B:709:THR:CG2	2:B:710:LYS:N	2.78	0.45
4:G:3047:TYR:C	4:G:3049:PRO:CD	2.90	0.45
4:G:3181:TYR:CD1	4:G:3181:TYR:C	2.94	0.45
1:C:1066:GLY:HA3	1:C:1071:TYR:CD2	2.52	0.45
4:G:3194:SER:OG	4:G:3196:LYS:HG3	2.15	0.45
2:D:1675:LEU:HD13	2:D:1675:LEU:C	2.41	0.45
3:E:855:ASP:OD1	3:E:864:TYR:HE2	2.00	0.45
4:F:2233:VAL:HG22	4:F:2251:LEU:HB2	1.97	0.45
1:A:55:HIS:C	1:A:55:HIS:HD1	2.25	0.45
2:D:1539:GLN:HB2	2:D:1545:LEU:CD2	2.46	0.45
2:D:1603:TYR:CE2	2:D:1604:TYR:CD1	3.05	0.45
3:E:868:LEU:HD22	3:E:875:MET:HE2	1.98	0.45
4:G:3120:GLN:O	4:G:3120:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:3156:SER:CB	4:G:3254:ALA:HB3	2.43	0.45
3:E:874:HIS:O	3:E:875:MET:HB2	2.17	0.45
2:B:560:TYR:OH	2:B:569:THR:HA	2.16	0.45
4:F:2120:GLN:O	4:F:2120:GLN:HG2	2.16	0.45
4:G:3168:GLY:O	4:G:3213:SER:N	2.50	0.45
4:G:3229:GLU:HB2	4:G:3231:LYS:HE3	1.98	0.45
2:D:1631:PRO:O	2:D:1718:ARG:HD2	2.15	0.45
1:A:161:ASN:ND2	1:A:177:SER:OG	2.48	0.45
1:C:1121:SER:C	1:C:1123:GLU:N	2.73	0.45
4:F:2012:CYS:HB2	4:F:2034:CYS:HA	1.99	0.45
4:F:2073:ILE:O	4:F:2075:GLU:N	2.50	0.45
4:F:2110:VAL:O	4:F:2111:VAL:HG13	2.17	0.45
4:G:3073:ILE:O	4:G:3075:GLU:N	2.50	0.45
4:F:2100:GLU:CD	4:F:2100:GLU:H	2.25	0.44
3:E:847:THR:O	3:E:850:ALA:N	2.44	0.44
4:F:2185:THR:HG22	4:F:2186:THR:N	2.32	0.44
2:D:1528:THR:O	2:D:1529:PHE:C	2.61	0.44
4:F:2005:VAL:O	4:F:2005:VAL:HG22	2.17	0.44
4:G:3030:PHE:CZ	4:G:3126:VAL:HG21	2.52	0.44
4:G:3100:GLU:H	4:G:3100:GLU:CD	2.25	0.44
1:A:118:PHE:CE1	1:A:135:PHE:HD2	2.34	0.44
1:A:144:ILE:HG13	1:A:145:ASN:N	2.33	0.44
4:F:2229:GLU:HB2	4:F:2231:LYS:HE3	1.99	0.44
1:A:125:LEU:C	1:A:127:SER:H	2.25	0.44
1:A:175:MET:CE	1:A:177:SER:HB2	2.48	0.44
2:B:620:LYS:HE3	2:B:620:LYS:HA	1.99	0.44
2:D:1632:VAL:O	2:D:1633:CYS:C	2.60	0.44
4:F:2181:TYR:CD1	4:F:2181:TYR:C	2.95	0.44
2:D:1536:TRP:CE2	2:D:1581:MET:HG3	2.52	0.44
4:G:3253:PHE:H	4:G:3253:PHE:HD1	1.65	0.44
1:C:1183:LYS:O	1:C:1187:GLU:HG3	2.18	0.44
1:C:1195:GLU:CG	1:C:1206:VAL:HG22	2.48	0.44
2:D:1553:THR:OG1	4:G:3064:SER:HB2	2.17	0.44
3:E:829:PHE:HE2	3:E:861:ASN:ND2	2.16	0.44
1:A:15:LEU:HA	1:A:78:LEU:HB3	1.99	0.44
1:A:198:HIS:CD2	1:A:199:LYS:H	2.36	0.44
1:C:1140:TYR:CD2	1:C:1141:PRO:HG3	2.53	0.44
4:F:2040:THR:HG21	4:F:2046:ALA:HB2	1.99	0.44
1:A:6:GLN:CG	1:A:100:GLY:H	2.31	0.44
1:A:13:ALA:O	1:A:107:LYS:N	2.50	0.44
2:B:568:ALA:HB1	2:B:581:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1193:THR:CG2	1:C:1208:SER:HB3	2.46	0.44
4:F:2112:GLY:HA3	4:F:2123:MET:HA	1.99	0.44
4:G:3070:SER:C	4:G:3072:LEU:N	2.76	0.44
4:G:3141:ARG:HG2	4:G:3166:VAL:CB	2.48	0.44
4:G:3185:THR:HG22	4:G:3186:THR:N	2.32	0.44
1:A:6:GLN:HG3	1:A:100:GLY:H	1.83	0.43
2:D:1522:CYS:HB2	2:D:1536:TRP:CH2	2.52	0.43
2:D:1572:VAL:CG2	2:D:1573:ASP:H	2.17	0.43
3:E:839:PHE:CD1	3:E:839:PHE:N	2.86	0.43
4:F:2152:PRO:HB2	4:F:2252:GLU:OE2	2.17	0.43
4:F:2168:GLY:O	4:F:2213:SER:N	2.51	0.43
4:F:2194:SER:OG	4:F:2196:LYS:HG3	2.17	0.43
4:G:3112:GLY:CA	4:G:3122:CYS:O	2.65	0.43
4:G:3175:PRO:HG3	4:G:3190:CYS:SG	2.57	0.43
1:A:91:GLY:O	2:B:603:TYR:HB2	2.18	0.43
1:C:1166:GLN:HB2	1:C:1173:TYR:CE1	2.53	0.43
1:C:1198:HIS:CD2	1:C:1199:LYS:H	2.35	0.43
4:F:2144:TYR:HB3	4:F:2239:GLY:O	2.18	0.43
4:G:3097:VAL:HA	4:G:3098:PRO:HD3	1.90	0.43
1:A:35:TRP:CE3	1:A:88:CYS:HB3	2.53	0.43
1:A:162:SER:O	1:A:175:MET:HA	2.18	0.43
1:C:1002:ILE:HG21	1:C:1093:THR:HB	1.99	0.43
4:G:3106:THR:HG23	4:G:3128:VAL:O	2.19	0.43
4:G:3131:ARG:NE	4:G:3131:ARG:CA	2.78	0.43
1:C:1062:PHE:CD2	1:C:1073:LEU:HD11	2.51	0.43
4:G:3175:PRO:O	4:G:3176:GLN:C	2.62	0.43
1:A:79:GLU:O	1:A:80:GLN:C	2.61	0.43
2:B:637:THR:O	2:B:637:THR:HG22	2.19	0.43
1:C:1089:GLN:HE21	1:C:1089:GLN:HB3	1.59	0.43
4:G:3014:ASP:O	4:G:3015:LYS:HB3	2.18	0.43
1:A:162:SER:OG	2:B:672:PRO:HG2	2.19	0.43
1:C:1210:ASN:C	1:C:1212:ASN:N	2.77	0.43
2:D:1642:THR:O	2:D:1643:LEU:HD23	2.18	0.43
4:F:2112:GLY:CA	4:F:2122:CYS:O	2.67	0.43
4:F:2194:SER:C	4:F:2196:LYS:N	2.75	0.43
1:A:11:LEU:HD23	1:A:104:LEU:HD21	2.01	0.43
1:A:66:GLY:HA3	1:A:71:TYR:CD2	2.53	0.43
4:F:2182:CYS:HB2	4:F:2234:ILE:HB	2.01	0.43
4:G:3210:ASN:O	4:G:3212:SER:N	2.51	0.43
4:G:3233:VAL:CG2	4:G:3251:LEU:HB2	2.49	0.43
2:B:523:LYS:HG2	2:B:578:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:568:ALA:HB1	2:B:581:MET:HE1	2.01	0.43
1:C:1015:LEU:HA	1:C:1078:LEU:HB3	2.00	0.43
4:G:3053:ILE:O	4:G:3054:CYS:C	2.62	0.43
1:A:31:ASN:O	1:A:50:TYR:HA	2.19	0.43
1:A:140:TYR:CD2	1:A:141:PRO:HG3	2.54	0.43
1:A:144:ILE:HG13	1:A:145:ASN:H	1.84	0.43
1:A:210:ASN:C	1:A:212:ASN:N	2.75	0.43
1:C:1031:ASN:O	1:C:1050:TYR:HA	2.19	0.43
1:C:1098:PHE:O	1:C:1099:GLY:O	2.37	0.43
3:E:843:PHE:HZ	3:E:872:GLY:HA3	1.84	0.43
4:G:3012:CYS:HB2	4:G:3034:CYS:HA	2.01	0.43
1:A:2:ILE:HD11	1:A:29:ILE:HG22	1.99	0.42
1:C:1143:ASP:OD1	3:E:878:LYS:HE2	2.19	0.42
2:D:1664:LEU:HD23	2:D:1686:VAL:HG21	2.00	0.42
4:F:2005:VAL:O	4:F:2005:VAL:HG13	2.18	0.42
4:F:2070:SER:OG	4:F:2076:ALA:HB3	2.19	0.42
4:G:3144:TYR:HB3	4:G:3239:GLY:O	2.19	0.42
1:A:14:SER:C	1:A:78:LEU:HD12	2.44	0.42
1:A:115:VAL:HA	1:A:135:PHE:O	2.19	0.42
2:B:534:MET:O	2:B:550:ILE:HA	2.19	0.42
2:D:1532:TYR:CD1	2:D:1532:TYR:N	2.87	0.42
4:F:2108:THR:HG23	4:F:2127:THR:HG23	2.01	0.42
4:G:3098:PRO:HB3	4:G:3100:GLU:OE1	2.19	0.42
2:B:602:TRP:CE2	4:F:2063:THR:HG22	2.54	0.42
1:C:1049:TYR:CZ	1:C:1053:ARG:HB3	2.53	0.42
1:C:1146:VAL:HG12	1:C:1147:LYS:N	2.35	0.42
4:F:2041:GLU:CB	4:F:2042:PRO:CD	2.97	0.42
4:F:2175:PRO:HG3	4:F:2190:CYS:SG	2.59	0.42
4:F:2210:ASN:O	4:F:2212:SER:N	2.52	0.42
4:G:3005:VAL:O	4:G:3005:VAL:HG22	2.18	0.42
4:G:3041:GLU:O	4:G:3043:PRO:CD	2.59	0.42
4:G:3138:ASN:ND2	4:G:3153:VAL:HG12	2.34	0.42
4:G:3141:ARG:HA	4:G:3166:VAL:HB	2.01	0.42
4:G:3152:PRO:HB2	4:G:3252:GLU:OE2	2.20	0.42
1:A:115:VAL:HG22	1:A:136:LEU:HG	2.02	0.42
2:B:587:THR:O	2:B:589:GLU:N	2.53	0.42
1:C:1135:PHE:CE1	2:D:1671:PHE:HE1	2.37	0.42
1:C:1144:ILE:HG13	1:C:1145:ASN:N	2.35	0.42
1:A:12:SER:HA	1:A:105:GLU:O	2.19	0.42
2:B:532:TYR:CD1	2:B:532:TYR:N	2.87	0.42
1:C:1005:THR:HG22	1:C:1006:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1015:LEU:HG	1:C:1106:ILE:HD12	2.01	0.42
2:D:1709:THR:CG2	2:D:1710:LYS:N	2.82	0.42
3:E:826:ASN:O	3:E:827:LEU:HD12	2.19	0.42
2:B:501:GLN:O	2:B:502:VAL:C	2.62	0.42
4:F:2135:VAL:HG13	4:F:2139:VAL:H	1.84	0.42
4:F:2138:ASN:ND2	4:F:2153:VAL:HG12	2.34	0.42
4:G:3198:ILE:C	4:G:3199:LEU:HD22	2.45	0.42
1:C:1175:MET:HE1	1:C:1177:SER:HB2	2.02	0.42
4:F:2198:ILE:C	4:F:2199:LEU:HD22	2.45	0.42
4:F:2226:PHE:H	4:F:2226:PHE:HD1	1.68	0.42
4:G:3005:VAL:O	4:G:3005:VAL:HG13	2.19	0.42
1:A:108:ARG:O	1:A:109:ALA:C	2.63	0.42
1:A:119:PRO:HB3	1:A:209:PHE:CE1	2.55	0.42
1:A:161:ASN:HD22	1:A:177:SER:HA	1.85	0.42
1:A:195:GLU:CG	1:A:206:VAL:HG22	2.50	0.42
1:C:1162:SER:OG	2:D:1672:PRO:HG2	2.20	0.42
2:D:1606:ASP:HB3	2:D:1607:TYR:HD1	1.85	0.42
4:F:2070:SER:C	4:F:2072:LEU:N	2.78	0.42
4:F:2131:ARG:NE	4:F:2131:ARG:CA	2.78	0.42
4:G:3108:THR:HG23	4:G:3127:THR:HG23	2.01	0.42
4:G:3226:PHE:H	4:G:3226:PHE:HD1	1.67	0.42
2:B:689:THR:O	2:B:691:SER:N	2.53	0.42
2:B:704:HIS:NE2	2:B:706:ALA:HB3	2.35	0.42
2:D:1539:GLN:O	2:D:1592:ALA:HB1	2.19	0.42
2:D:1547:TRP:CZ2	2:D:1550:ILE:HG22	2.55	0.42
2:D:1602:TRP:CE2	4:G:3063:THR:HG22	2.55	0.42
2:D:1650:TYR:CZ	2:D:1655:VAL:HG11	2.54	0.42
4:F:2030:PHE:HD1	4:F:2095:LEU:HD23	1.85	0.42
4:G:3241:SER:HB2	4:G:3242:PRO:HA	2.02	0.42
2:D:1512:VAL:CG1	2:D:1513:ARG:N	2.83	0.41
2:D:1587:THR:O	2:D:1589:GLU:N	2.53	0.41
2:D:1651:PHE:CD2	2:D:1651:PHE:C	2.98	0.41
4:F:2062:CYS:O	4:F:2063:THR:C	2.63	0.41
4:F:2066:ALA:C	4:F:2067:VAL:HG13	2.45	0.41
4:G:3109:PHE:CD1	4:G:3109:PHE:O	2.73	0.41
1:A:40:PRO:C	1:A:42:GLY:N	2.78	0.41
4:F:2026:THR:C	4:F:2027:GLU:HG3	2.45	0.41
4:G:3030:PHE:HD1	4:G:3095:LEU:HD23	1.85	0.41
4:G:3041:GLU:CB	4:G:3042:PRO:CD	2.97	0.41
1:A:5:THR:HG22	1:A:6:GLN:N	2.35	0.41
1:C:1040:PRO:C	1:C:1042:GLY:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1135:PHE:CE1	2:D:1671:PHE:CE1	3.08	0.41
1:C:1144:ILE:HG13	1:C:1145:ASN:H	1.86	0.41
3:E:847:THR:C	3:E:850:ALA:H	2.28	0.41
1:A:1:ASP:N	1:A:95:PRO:HD2	2.34	0.41
2:B:537:VAL:HG13	2:B:546:GLU:O	2.20	0.41
2:D:1689:THR:O	2:D:1691:SER:N	2.52	0.41
4:F:2014:ASP:O	4:F:2015:LYS:HB3	2.21	0.41
4:F:2031:THR:HA	4:F:2093:ILE:O	2.20	0.41
4:G:3059:THR:HG22	4:G:3060:SER:N	2.35	0.41
4:G:3133:SER:HB2	4:G:3141:ARG:O	2.20	0.41
4:G:3135:VAL:HG13	4:G:3139:VAL:H	1.85	0.41
4:G:3230:SER:O	4:G:3231:LYS:HD2	2.21	0.41
1:A:39:LYS:HD2	1:A:84:ALA:HB2	2.02	0.41
2:B:522:CYS:HB2	2:B:536:TRP:HH2	1.86	0.41
2:B:561:ASN:OD1	2:B:561:ASN:C	2.63	0.41
2:B:606:ASP:HB3	2:B:607:TYR:HD1	1.85	0.41
2:B:642:THR:C	2:B:643:LEU:HD23	2.46	0.41
4:G:3107:GLN:HB2	4:G:3128:VAL:CG2	2.50	0.41
4:G:3194:SER:C	4:G:3196:LYS:N	2.74	0.41
2:D:1501:GLN:O	2:D:1502:VAL:C	2.63	0.41
4:F:2066:ALA:O	4:F:2067:VAL:CG1	2.68	0.41
4:G:3175:PRO:HG2	4:G:3181:TYR:CA	2.50	0.41
1:A:15:LEU:HG	1:A:106:ILE:HD12	2.03	0.41
1:A:52:SER:HB3	1:A:64:GLY:O	2.21	0.41
1:A:89:GLN:HE21	1:A:89:GLN:HB3	1.59	0.41
1:A:195:GLU:HG3	1:A:206:VAL:HG22	2.02	0.41
2:B:512:VAL:CG1	2:B:513:ARG:N	2.84	0.41
2:B:627:TYR:HA	2:B:628:PRO:HD3	1.89	0.41
1:C:1039:LYS:HD2	1:C:1084:ALA:HB2	2.03	0.41
1:C:1115:VAL:HG22	1:C:1136:LEU:HG	2.02	0.41
1:C:1118:PHE:CE1	1:C:1135:PHE:CD2	3.08	0.41
2:D:1637:THR:HG22	2:D:1637:THR:O	2.20	0.41
4:F:2020:ALA:HA	4:F:2125:THR:O	2.20	0.41
4:F:2109:PHE:CD1	4:F:2109:PHE:O	2.74	0.41
4:F:2175:PRO:O	4:F:2176:GLN:C	2.62	0.41
4:G:3034:CYS:O	4:G:3088:LEU:HB3	2.20	0.41
1:A:2:ILE:O	1:A:2:ILE:CG1	2.44	0.41
2:B:650:TYR:CZ	2:B:655:VAL:HG11	2.55	0.41
1:C:1035:TRP:HD1	1:C:1048:ILE:HG22	1.85	0.41
2:D:1551:ILE:O	2:D:1551:ILE:HG23	2.21	0.41
2:D:1660:ASN:ND2	2:D:1699:THR:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:842:THR:HG23	3:E:844:GLU:N	2.35	0.41
4:G:3199:LEU:HA	4:G:3200:PRO:HD2	1.90	0.41
1:A:79:GLU:HB2	1:A:82:ASP:OD2	2.21	0.41
1:A:80:GLN:C	1:A:82:ASP:H	2.29	0.41
2:B:551:ILE:HG23	2:B:551:ILE:O	2.21	0.41
2:B:572:VAL:CG2	2:B:573:ASP:H	2.15	0.41
2:B:637:THR:O	2:B:638:GLY:O	2.39	0.41
2:B:642:THR:O	2:B:643:LEU:HD23	2.20	0.41
1:C:1061:ARG:NH1	1:C:1082:ASP:OD2	2.53	0.41
1:C:1115:VAL:HA	1:C:1135:PHE:O	2.21	0.41
1:C:1136:LEU:HD21	1:C:1196:ALA:HB2	2.02	0.41
1:C:1150:ILE:HD11	1:C:1179:LEU:CD2	2.39	0.41
2:D:1561:ASN:OD1	2:D:1561:ASN:C	2.64	0.41
2:D:1620:LYS:HE3	2:D:1620:LYS:HA	2.02	0.41
4:F:2030:PHE:CZ	4:F:2126:VAL:HG21	2.56	0.41
4:F:2032:LEU:HB3	4:F:2093:ILE:HB	2.03	0.41
4:F:2053:ILE:O	4:F:2054:CYS:C	2.64	0.41
4:F:2060:SER:OG	4:F:2061:SER:N	2.50	0.41
4:F:2098:PRO:O	4:F:2099:ILE:C	2.62	0.41
4:F:2233:VAL:CG2	4:F:2251:LEU:HB2	2.50	0.41
4:G:3026:THR:C	4:G:3027:GLU:HG3	2.46	0.41
4:G:3034:CYS:O	4:G:3035:PRO:O	2.38	0.41
4:G:3098:PRO:O	4:G:3099:ILE:C	2.64	0.41
4:G:3101:LYS:O	4:G:3102:PHE:C	2.63	0.41
1:A:15:LEU:HG	1:A:106:ILE:CD1	2.51	0.41
1:A:146:VAL:HG12	1:A:147:LYS:N	2.35	0.41
2:B:657:LEU:HD23	2:B:702:VAL:HG22	1.97	0.41
1:C:1015:LEU:HG	1:C:1106:ILE:CD1	2.51	0.41
1:C:1030:SER:O	1:C:1031:ASN:HB2	2.21	0.41
4:F:2044:THR:OG1	4:F:2052:GLN:HB2	2.21	0.41
4:F:2240:GLY:O	4:F:2241:SER:HB3	2.21	0.41
4:F:2241:SER:HB2	4:F:2242:PRO:HA	2.03	0.41
1:C:1006:GLN:CG	1:C:1100:GLY:H	2.32	0.40
2:D:1602:TRP:CD1	4:G:3063:THR:HG22	2.56	0.40
4:G:3044:THR:OG1	4:G:3052:GLN:HB2	2.20	0.40
4:G:3073:ILE:HA	4:G:3074:PRO:HD2	1.81	0.40
4:G:3113:CYS:O	4:G:3121:SER:HA	2.21	0.40
4:G:3201:LYS:HE3	4:G:3202:LEU:H	1.79	0.40
1:C:1006:GLN:HG3	1:C:1100:GLY:H	1.86	0.40
1:C:1161:ASN:ND2	1:C:1177:SER:OG	2.54	0.40
2:D:1602:TRP:CD1	2:D:1602:TRP:N	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2034:CYS:O	4:F:2035:PRO:O	2.39	0.40
4:F:2187:LEU:HB2	4:F:2246:HIS:HD2	1.86	0.40
4:G:3032:LEU:HB3	4:G:3093:ILE:HB	2.03	0.40
1:C:1052:SER:HB3	1:C:1064:GLY:O	2.21	0.40
3:E:845:GLU:O	3:E:847:THR:N	2.54	0.40
4:F:2113:CYS:O	4:F:2121:SER:HA	2.21	0.40
4:F:2113:CYS:N	4:F:2122:CYS:O	2.52	0.40
4:F:2154:LYS:HA	4:F:2252:GLU:HB2	2.04	0.40
4:G:3062:CYS:O	4:G:3063:THR:C	2.64	0.40
4:G:3240:GLY:O	4:G:3241:SER:HB3	2.21	0.40
1:A:30:SER:O	1:A:31:ASN:HB2	2.21	0.40
1:A:32:TYR:CE2	1:A:50:TYR:HE1	2.39	0.40
2:B:517:SER:HB2	2:B:584:ALA:HA	2.03	0.40
2:B:682:LEU:C	2:B:682:LEU:CD2	2.94	0.40
1:C:1189:HIS:HB3	1:C:1190:ASN:H	1.78	0.40
2:D:1586:LEU:HD23	2:D:1590:ASP:OD2	2.21	0.40
4:F:2141:ARG:HG2	4:F:2166:VAL:CG2	2.51	0.40
4:G:3003:PRO:C	4:G:3004:LEU:HD12	2.46	0.40
4:G:3102:PHE:CB	4:G:3103:PRO:HD2	2.51	0.40
4:G:3208:GLN:O	4:G:3217:ALA:HA	2.21	0.40
2:B:590:ASP:O	2:B:591:SER:C	2.62	0.40
4:F:2175:PRO:HG2	4:F:2181:TYR:CA	2.49	0.40
4:G:3009:VAL:HG13	4:G:3031:THR:HB	2.03	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	211/213 (99%)	165 (78%)	40 (19%)	6 (3%)	4	20
1	C	211/213 (99%)	166 (79%)	37 (18%)	8 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	216/218 (99%)	177 (82%)	26 (12%)	13 (6%)	1	7
2	D	216/218 (99%)	177 (82%)	26 (12%)	13 (6%)	1	7
3	E	59/61 (97%)	44 (75%)	9 (15%)	6 (10%)	0	3
4	F	250/254 (98%)	177 (71%)	47 (19%)	26 (10%)	0	2
4	G	250/254 (98%)	173 (69%)	50 (20%)	27 (11%)	0	2
All	All	1413/1431 (99%)	1079 (76%)	235 (17%)	99 (7%)	1	5

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	27	GLN
2	B	575	SER
2	B	633	CYS
1	C	1017	ASP
1	C	1027	GLN
2	D	1574	LYS
2	D	1575	SER
3	E	859	LYS
3	E	870	ASP
4	F	2005	VAL
4	F	2049	PRO
4	F	2089	ASP
4	F	2120	GLN
4	F	2147	ASP
4	F	2200	PRO
4	F	2204	GLU
4	F	2211	ALA
4	G	3005	VAL
4	G	3035	PRO
4	G	3049	PRO
4	G	3089	ASP
4	G	3120	GLN
4	G	3200	PRO
4	G	3204	GLU
4	G	3211	ALA
1	A	211	ARG
2	B	574	LYS
2	B	588	SER
2	B	606	ASP

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Mol	Chain	Res	Type
2	B	637	THR
2	B	638	GLY
2	B	655	VAL
2	B	690	SER
1	C	1099	GLY
1	C	1211	ARG
2	D	1588	SER
2	D	1606	ASP
2	D	1633	CYS
2	D	1637	THR
2	D	1638	GLY
2	D	1655	VAL
2	D	1690	SER
3	E	830	ALA
3	E	873	ASN
4	F	2035	PRO
4	F	2074	PRO
4	F	2111	VAL
4	F	2131	ARG
4	F	2194	SER
4	F	2210	ASN
4	G	3038	ALA
4	G	3074	PRO
4	G	3111	VAL
4	G	3131	ARG
4	G	3147	ASP
4	G	3194	SER
4	G	3210	ASN
1	A	99	GLY
1	A	138	ASN
2	B	522	CYS
1	C	1138	ASN
2	D	1522	CYS
4	F	2038	ALA
4	F	2116	GLY
4	F	2133	SER
4	F	2217	ALA
4	F	2223	LYS
4	G	3116	GLY
4	G	3133	SER
4	G	3217	ALA
4	G	3223	LYS

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Mol	Chain	Res	Type
1	A	81	GLU
2	B	653	GLU
2	B	695	SER
1	C	1191	SER
2	D	1543	LYS
2	D	1695	SER
4	F	2088	LEU
4	F	2197	ASP
4	G	3088	LEU
4	G	3197	ASP
4	G	3222	LYS
2	B	543	LYS
1	C	1015	LEU
1	C	1081	GLU
2	D	1653	GLU
4	F	2184	GLY
4	F	2222	LYS
3	E	875	MET
4	F	2048	SER
4	F	2100	GLU
4	G	3048	SER
4	G	3071	SER
4	G	3158	GLU
4	G	3184	GLY
3	E	832	GLY
4	F	2226	PHE
4	G	3226	PHE

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	191/191 (100%)	172 (90%)	19 (10%)	7	29
1	C	191/191 (100%)	171 (90%)	20 (10%)	6	26
2	B	188/188 (100%)	163 (87%)	25 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	188/188 (100%)	163 (87%)	25 (13%)	4	17
3	E	47/47 (100%)	43 (92%)	4 (8%)	10	35
4	F	214/215 (100%)	201 (94%)	13 (6%)	17	46
4	G	214/215 (100%)	202 (94%)	12 (6%)	19	49
All	All	1233/1235 (100%)	1115 (90%)	118 (10%)	8	30

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	6	GLN
1	A	7	THR
1	A	19	VAL
1	A	46	LEU
1	A	48	ILE
1	A	69	THR
1	A	70	ASP
1	A	89	GLN
1	A	94	LEU
1	A	104	LEU
1	A	108	ARG
1	A	116	SER
1	A	138	ASN
1	A	165	ASP
1	A	171	SER
1	A	176	SER
1	A	197	THR
1	A	205	ILE
2	B	504	LEU
2	B	505	GLN
2	B	541	HIS
2	B	567	LYS
2	B	569	THR
2	B	581	MET
2	B	588	SER
2	B	598	ARG
2	B	601	THR
2	B	603	TYR
2	B	604	TYR
2	B	606	ASP
2	B	610	GLN

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Mol	Chain	Res	Type
2	B	620	LYS
2	B	632	VAL
2	B	633	CYS
2	B	648	LYS
2	B	657	LEU
2	B	664	LEU
2	B	665	SER
2	B	670	THR
2	B	676	GLN
2	B	689	THR
2	B	699	THR
2	B	713	LYS
1	C	1002	ILE
1	C	1007	THR
1	C	1019	VAL
1	C	1046	LEU
1	C	1048	ILE
1	C	1069	THR
1	C	1070	ASP
1	C	1085	THR
1	C	1089	GLN
1	C	1094	LEU
1	C	1104	LEU
1	C	1108	ARG
1	C	1113	PRO
1	C	1116	SER
1	C	1138	ASN
1	C	1165	ASP
1	C	1171	SER
1	C	1176	SER
1	C	1197	THR
1	C	1205	ILE
2	D	1504	LEU
2	D	1505	GLN
2	D	1541	HIS
2	D	1567	LYS
2	D	1569	THR
2	D	1581	MET
2	D	1598	ARG
2	D	1601	THR
2	D	1603	TYR
2	D	1604	TYR

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Mol	Chain	Res	Type
2	D	1606	ASP
2	D	1610	GLN
2	D	1620	LYS
2	D	1632	VAL
2	D	1633	CYS
2	D	1648	LYS
2	D	1657	LEU
2	D	1664	LEU
2	D	1665	SER
2	D	1670	THR
2	D	1676	GLN
2	D	1681	THR
2	D	1689	THR
2	D	1699	THR
2	D	1713	LYS
3	E	831	ASP
3	E	842	THR
3	E	865	THR
3	E	876	ASN
4	F	2010	VAL
4	F	2029	HIS
4	F	2040	THR
4	F	2053	ILE
4	F	2111	VAL
4	F	2127	THR
4	F	2131	ARG
4	F	2190	CYS
4	F	2201	LYS
4	F	2204	GLU
4	F	2235	ILE
4	F	2237	CYS
4	F	2253	PHE
4	G	3010	VAL
4	G	3029	HIS
4	G	3040	THR
4	G	3053	ILE
4	G	3111	VAL
4	G	3131	ARG
4	G	3190	CYS
4	G	3201	LYS
4	G	3204	GLU
4	G	3235	ILE

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Mol	Chain	Res	Type
4	G	3237	CYS
4	G	3253	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	38	GLN
1	A	77	ASN
1	A	80	GLN
1	A	89	GLN
1	A	137	ASN
1	A	161	ASN
2	B	505	GLN
2	B	539	GLN
2	B	541	HIS
2	B	660	ASN
2	B	669	HIS
2	B	676	GLN
1	C	1031	ASN
1	C	1038	GLN
1	C	1077	ASN
1	C	1080	GLN
1	C	1089	GLN
1	C	1137	ASN
1	C	1161	ASN
2	D	1505	GLN
2	D	1539	GLN
2	D	1660	ASN
2	D	1669	HIS
2	D	1676	GLN
3	E	861	ASN
3	E	876	ASN
4	F	2007	ASN
4	F	2029	HIS
4	F	2050	ASN
4	F	2137	ASN
4	F	2138	ASN
4	F	2178	ASN
4	F	2180	GLN
4	F	2191	ASN
4	G	3007	ASN

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Mol	Chain	Res	Type
4	G	3029	HIS
4	G	3050	ASN
4	G	3129	GLN
4	G	3137	ASN
4	G	3138	ASN
4	G	3178	ASN
4	G	3180	GLN
4	G	3191	ASN
4	G	3246	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	213/213 (100%)	-1.11	0 100 100	24, 54, 77, 89	0
1	C	213/213 (100%)	-1.12	0 100 100	23, 54, 76, 89	0
2	B	218/218 (100%)	-1.14	0 100 100	16, 50, 78, 102	0
2	D	218/218 (100%)	-1.12	0 100 100	16, 50, 78, 102	0
3	E	61/61 (100%)	-1.04	0 100 100	48, 77, 95, 103	0
4	F	252/254 (99%)	-0.65	0 100 100	67, 106, 142, 150	0
4	G	252/254 (99%)	-0.65	0 100 100	67, 106, 139, 150	0
All	All	1427/1431 (99%)	-0.95	0 100 100	16, 68, 134, 150	0

There are no RSRZ outliers to report.

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	CD	D	4002	1/1	0.99	0.06	115,115,115,115	0
5	CD	B	4001	1/1	1.00	0.03	111,111,111,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.