



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:10 AM EDT

PDB ID : 8KA1 / pdb_00008ka1
Title : Crystal structure of Vibrio vulnificus RID-dependent transforming NADase domain (RDTND)/calmodulin-binding domain of Rho inactivation domain (RID-CBD) complexed with Ca²⁺-free calmodulin
Authors : Lee, Y.; Choi, S.; Hwang, J.; Kim, M.H.
Deposited on : 2023-08-02
Resolution : 2.82 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:

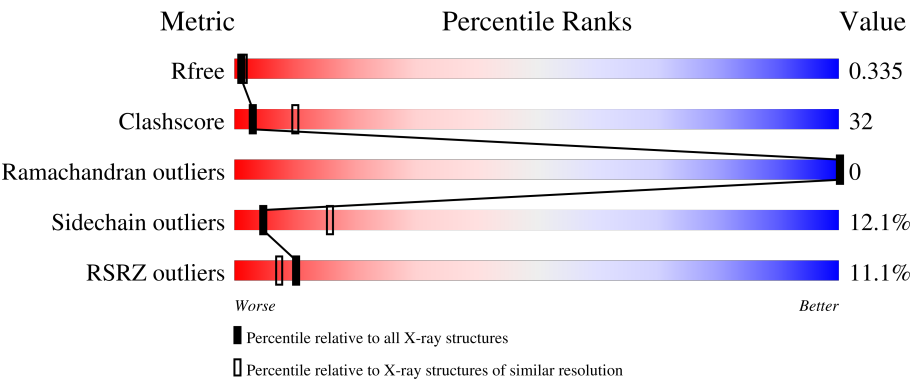
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	416	13% 53% 37% 6%
1	C	416	7% 56% 33% 8%
1	E	416	9% 50% 41% 5%
1	G	416	8% 60% 29% 8%
2	B	151	14% 49% 36% 10% 5%

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Mol	Chain	Length	Quality of chain
2	D	151	12% 35% 45% 8% 12%
2	F	151	9% 52% 37% 7% 5%
2	H	151	17% 48% 37% 7% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17066 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 RDTND-RID CBD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	Se	0	0	0
			3234	2042	551	636	5			
1	C	384	Total	C	N	O	Se	0	0	0
			3077	1947	523	602	5			
1	E	404	Total	C	N	O	Se	0	0	0
			3234	2042	551	636	5			
1	G	384	Total	C	N	O	Se	0	0	0
			3077	1947	523	602	5			

- Molecule 2 is a protein called Calmodulin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	Se	0	0	0
			1134	696	183	246	9			
2	D	133	Total	C	N	O	Se	0	0	0
			1058	653	170	226	9			
2	F	144	Total	C	N	O	Se	0	0	0
			1134	696	183	246	9			
2	H	139	Total	C	N	O	Se	0	0	0
			1097	675	177	236	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	cloning artifact	UNP P0DP24
B	0	ALA	-	cloning artifact	UNP P0DP24
B	124	GLN	GLU	conflict	UNP P0DP24
D	-1	GLY	-	cloning artifact	UNP P0DP24
D	0	ALA	-	cloning artifact	UNP P0DP24
D	124	GLN	GLU	conflict	UNP P0DP24
F	-1	GLY	-	cloning artifact	UNP P0DP24
F	0	ALA	-	cloning artifact	UNP P0DP24

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Chain	Residue	Modelled	Actual	Comment	Reference
F	124	GLN	GLU	conflict	UNP P0DP24
H	-1	GLY	-	cloning artifact	UNP P0DP24
H	0	ALA	-	cloning artifact	UNP P0DP24
H	124	GLN	GLU	conflict	UNP P0DP24

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	3	Total Mg 3 3	0	0

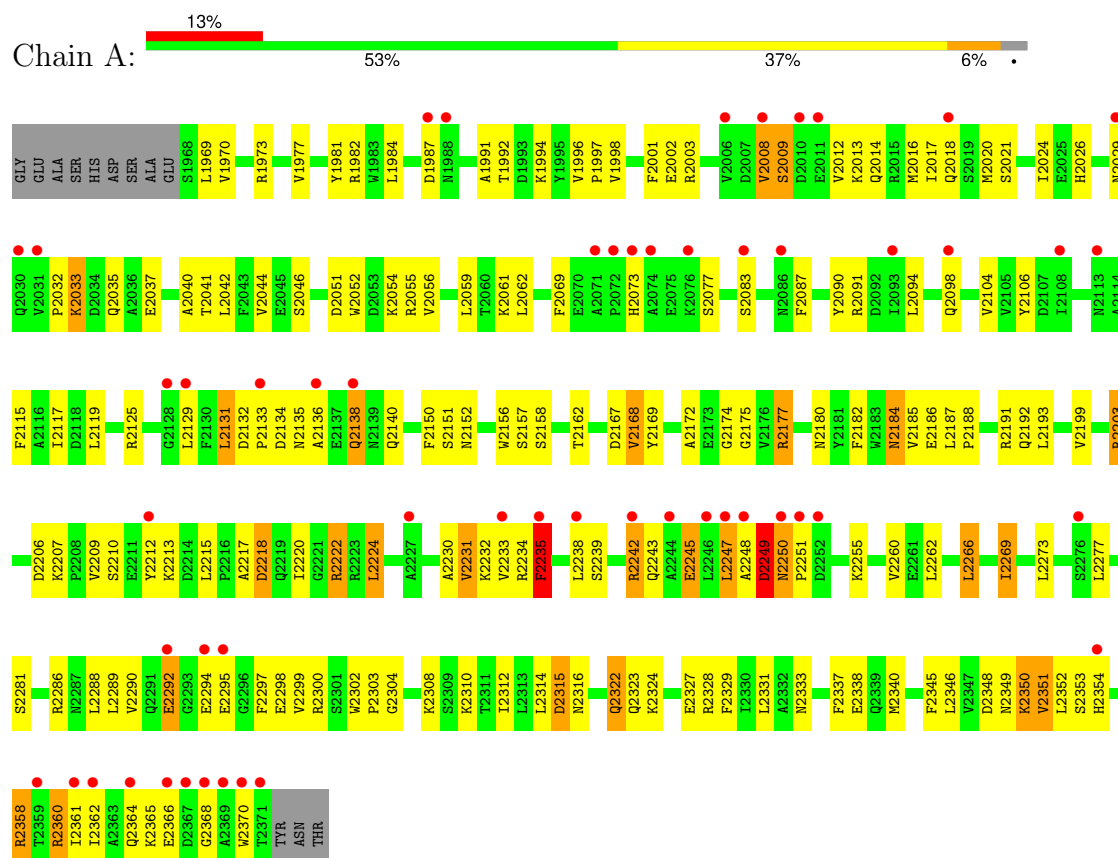
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	E	6	Total O 6 6	0	0
4	F	2	Total O 2 2	0	0
4	G	3	Total O 3 3	0	0
4	H	2	Total O 2 2	0	0

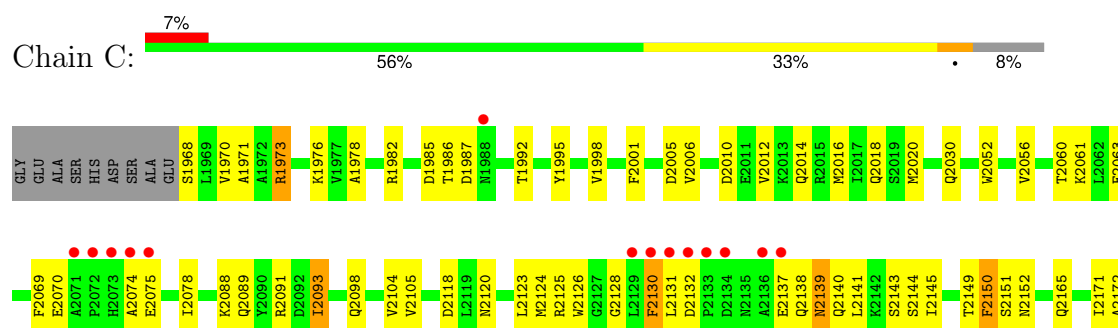
3 Residue-property plots [i](#)

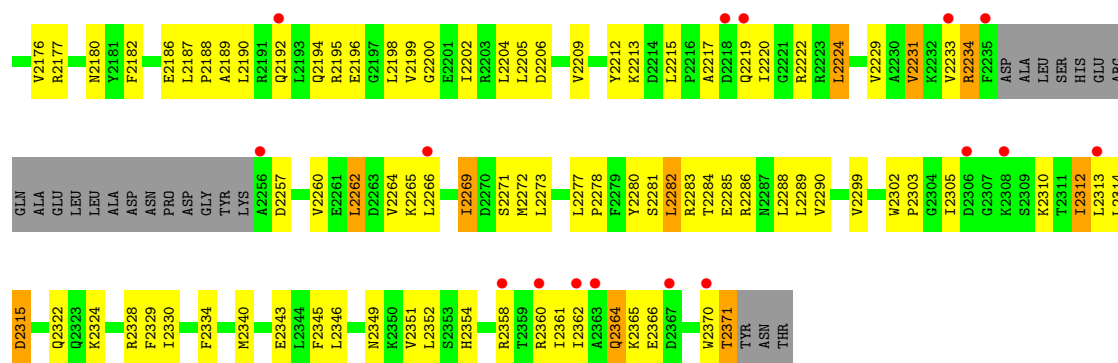
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

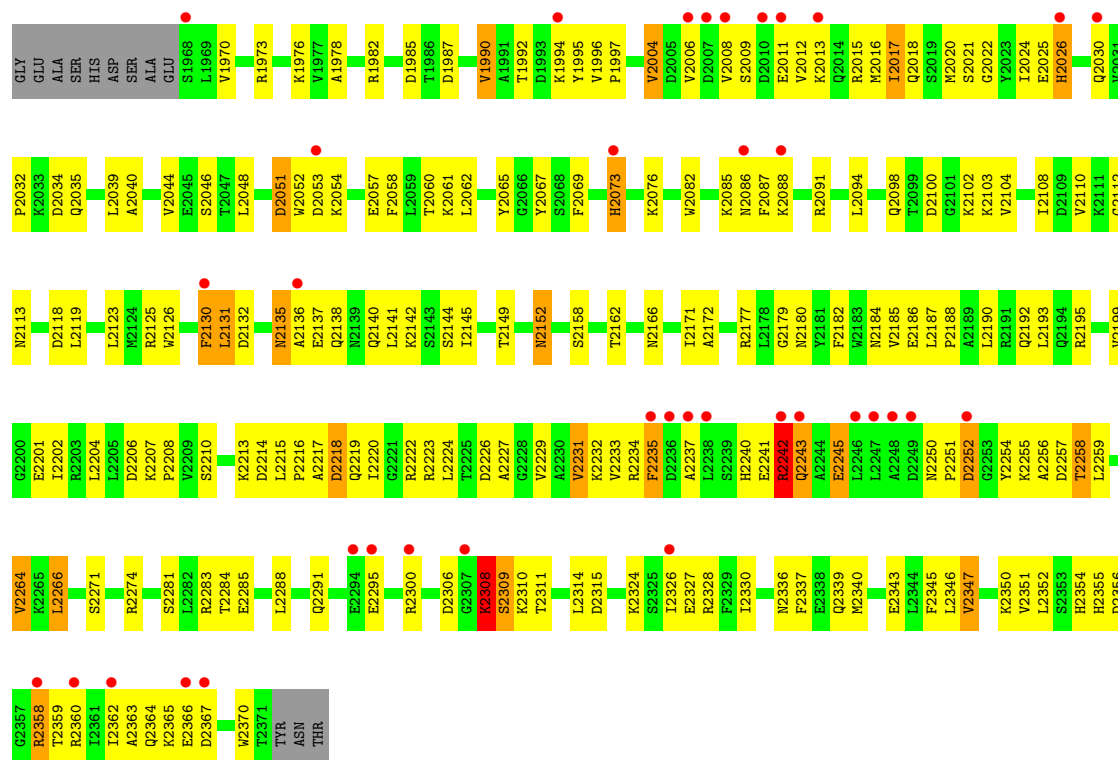


• Molecule 1: RDTND-RID CBD

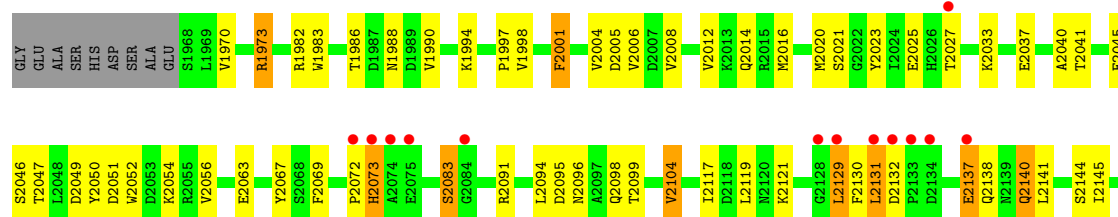


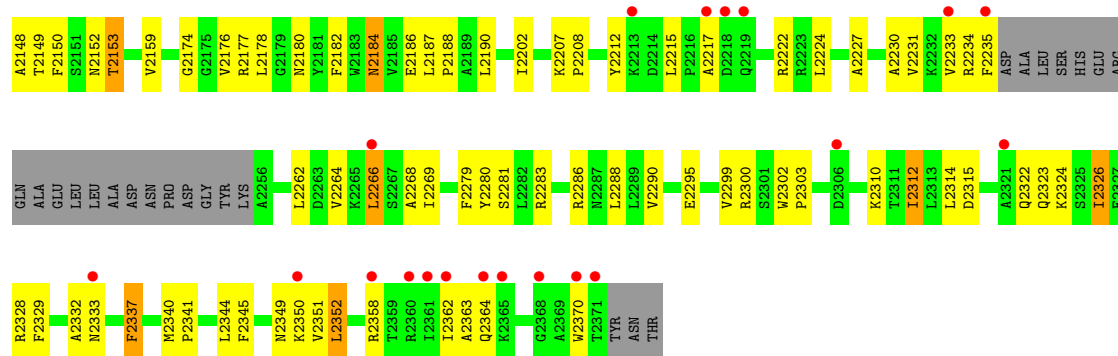


• Molecule 1: RDTND-RID CBD

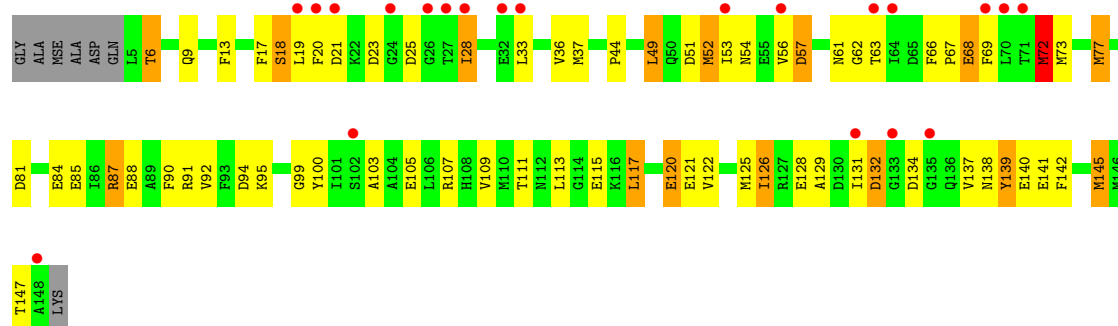


• Molecule 1: RDTND-RID CBD

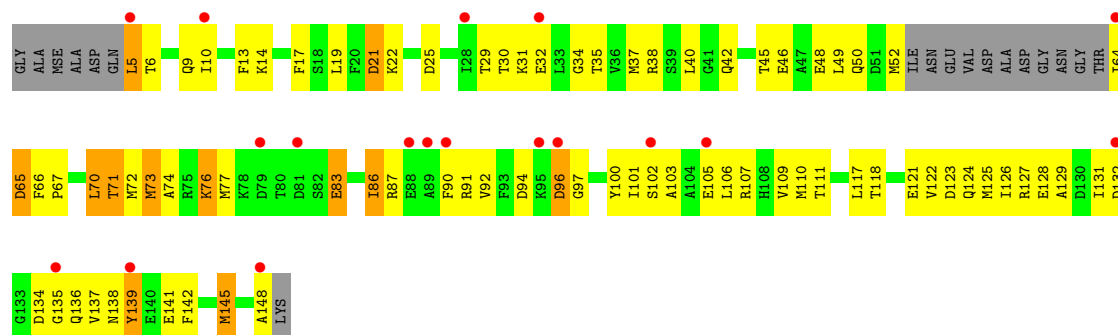




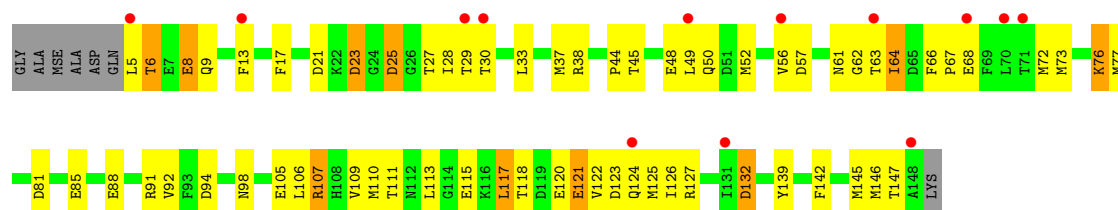
• Molecule 2: Calmodulin-2



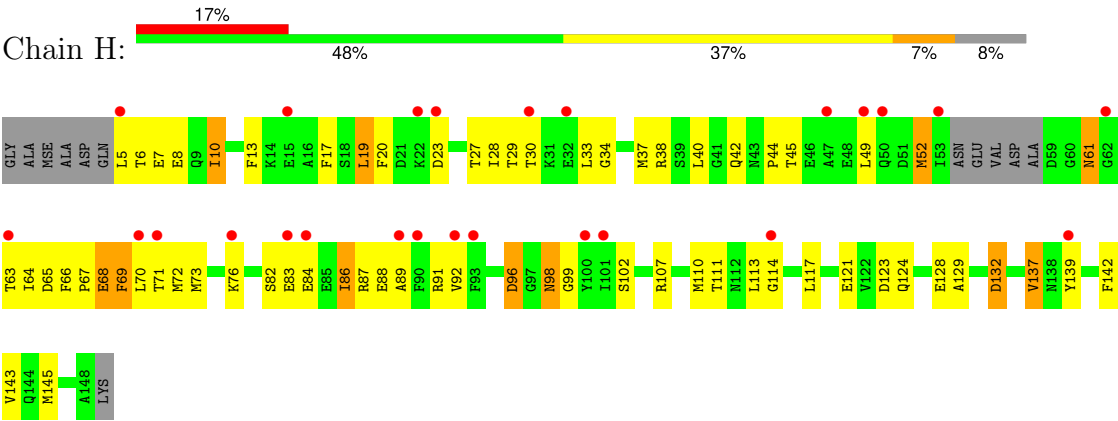
• Molecule 2: Calmodulin-2



• Molecule 2: Calmodulin-2



● Molecule 2: Calmodulin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.03Å 88.08Å 136.95Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	49.53 – 2.82 49.53 – 2.82	Depositor EDS
% Data completeness (in resolution range)	89.3 (49.53-2.82) 89.3 (49.53-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.271 , 0.342 0.272 , 0.335	Depositor DCC
R_{free} test set	2678 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17066	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9676e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.88	0/3295	1.05	3/4457 (0.1%)
1	C	0.88	1/3134 (0.0%)	1.01	0/4237
1	E	0.87	0/3295	1.02	3/4457 (0.1%)
1	G	0.87	0/3134	1.02	0/4237
2	B	0.95	0/1137	1.07	1/1512 (0.1%)
2	D	0.88	0/1060	1.07	2/1405 (0.1%)
2	F	0.93	1/1137 (0.1%)	1.06	1/1512 (0.1%)
2	H	0.87	0/1099	1.08	0/1458
All	All	0.88	2/17291 (0.0%)	1.04	10/23275 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2078	ILE	C-O	-5.69	1.17	1.24
2	F	21	ASP	CG-OD1	5.03	1.34	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2235	PHE	CB-CA-C	9.14	123.52	111.82
1	E	2308	LYS	N-CA-C	9.08	121.53	110.91
2	D	21	ASP	CA-CB-CG	7.15	119.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2235	PHE	CA-CB-CG	6.81	120.61	113.80
1	E	2100	ASP	N-CA-C	-6.52	105.96	114.04
1	E	2252	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	2249	ASP	N-CA-C	-5.76	106.30	113.15
2	D	21	ASP	CB-CA-C	5.29	120.51	112.00
2	B	72	MSE	CB-CG-SE	-5.19	97.14	112.70
2	F	27	THR	CA-CB-OG1	-5.06	102.00	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	2242	ARG	Sidechain

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	3234	0	3130	213	0
1	C	3077	0	2986	152	0
1	E	3234	0	3130	223	0
1	G	3077	0	2986	150	0
2	B	1134	0	1065	106	0
2	D	1058	0	1000	104	0
2	F	1134	0	1065	72	0
2	H	1097	0	1034	106	0
3	F	3	0	0	0	0
4	A	3	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	0	0
4	E	6	0	0	3	0
4	F	2	0	0	0	0
4	G	3	0	0	3	0
4	H	2	0	0	0	0
All	All	17066	0	16396	1061	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 32.

All (1061) 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:G:2129:LEU:HD13	1:G:2129:LEU:O	1.22	1.35
1:A:2250:ASN:HB2	1:A:2251:PRO:CD	1.57	1.25
1:A:2032:PRO:HB2	1:A:2035:GLN:CG	1.67	1.23
1:E:2326:ILE:HD11	1:E:2346:LEU:CB	1.74	1.17
1:A:2250:ASN:CB	1:A:2251:PRO:HD3	1.75	1.16
1:C:2329:PHE:CD2	1:C:2362:ILE:HD11	1.81	1.14
1:A:1996:VAL:CG2	1:A:2052:TRP:CE3	2.30	1.14
2:B:69:PHE:CZ	2:B:73:MSE:HE3	1.83	1.12
2:B:138:ASN:HD22	2:B:141:GLU:HG3	1.09	1.12
2:D:10:ILE:HG12	2:D:70:LEU:HD11	1.31	1.11
2:H:52:MSE:HG3	2:H:72:MSE:SE	2.00	1.11
1:A:2032:PRO:CB	1:A:2035:GLN:HG3	1.79	1.11
2:B:56:VAL:HG21	2:B:68:GLU:HG2	1.27	1.11
1:E:2177:ARG:HB2	1:E:2180:ASN:ND2	1.64	1.11
1:G:2264:VAL:HG11	2:H:92:VAL:HG11	1.26	1.10
1:A:2032:PRO:HB2	1:A:2035:GLN:HG3	1.26	1.09
2:H:10:ILE:HG23	2:H:70:LEU:HD11	1.29	1.09
2:D:30:THR:HG22	2:D:64:ILE:CG1	1.84	1.07
2:B:52:MSE:HE2	2:B:72:MSE:HB3	1.37	1.06
1:A:1996:VAL:HG21	1:A:2052:TRP:CE3	1.92	1.05
1:E:2132:ASP:H	1:E:2138:GLN:NE2	1.55	1.05
1:G:2016:MSE:CE	1:G:2145:ILE:HD11	1.86	1.05
2:B:52:MSE:O	2:B:56:VAL:HG12	1.55	1.04
1:C:2264:VAL:HG11	2:D:92:VAL:HG21	1.40	1.03
1:E:2326:ILE:CD1	1:E:2346:LEU:HB2	1.88	1.03
1:A:2020:MSE:CE	1:A:2119:LEU:HB3	1.87	1.03
2:D:10:ILE:CG2	2:D:70:LEU:HD21	1.89	1.03
2:D:37:MSE:HE3	2:D:73:MSE:HE2	1.37	1.03
1:E:2365:LYS:O	1:E:2366:GLU:HG2	1.59	1.02
2:D:10:ILE:HG23	2:D:70:LEU:HD21	1.03	1.02
1:E:2032:PRO:HB2	1:E:2035:GLN:HB2	1.41	1.02
1:E:2250:ASN:HB3	1:E:2251:PRO:HD3	1.41	1.02
2:D:30:THR:HG22	2:D:64:ILE:HG12	1.43	1.01
1:G:2129:LEU:HD12	1:G:2130:PHE:CE1	1.96	1.01
1:G:2328:ARG:NH2	2:H:40:LEU:HD23	1.76	1.00
2:H:10:ILE:HG23	2:H:70:LEU:CD1	1.90	1.00
2:B:44:PRO:CG	2:B:49:LEU:HD11	1.91	0.99
1:E:2013:LYS:O	1:E:2017:ILE:HG13	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2272:MSE:HE2	2:D:86:ILE:HG21	1.42	0.99
1:C:2343:GLU:CD	1:E:2358:ARG:HG2	1.87	0.99
1:G:2290:VAL:HG22	1:G:2299:VAL:HG22	1.42	0.99
1:A:1996:VAL:HG22	1:A:2052:TRP:CE3	1.98	0.98
1:A:2210:SER:O	1:A:2213:LYS:HG2	1.63	0.98
1:E:2193:LEU:HB3	1:E:2199:VAL:HG23	1.45	0.98
2:H:20:PHE:HB2	2:H:28:ILE:HD13	1.46	0.97
1:A:2033:LYS:HD3	1:A:2033:LYS:H	1.28	0.97
1:E:2004:VAL:CG1	1:E:2144:SER:HA	1.95	0.96
2:H:69:PHE:CE2	2:H:73:MSE:HE3	2.00	0.96
1:A:2020:MSE:HE1	1:A:2119:LEU:HB3	1.48	0.96
1:E:2314:LEU:HD21	1:E:2326:ILE:HD12	1.48	0.95
2:B:37:MSE:HG2	2:B:73:MSE:CE	1.95	0.95
2:F:52:MSE:HB3	2:F:72:MSE:SE	2.16	0.95
1:C:2343:GLU:OE1	1:E:2358:ARG:HG2	1.67	0.95
2:D:10:ILE:HG23	2:D:70:LEU:CD2	1.96	0.94
1:E:2132:ASP:H	1:E:2138:GLN:HE21	1.01	0.94
2:B:91:ARG:CG	2:B:139:TYR:HE2	1.81	0.94
1:A:2032:PRO:CG	1:A:2035:GLN:HG3	1.97	0.94
1:C:2264:VAL:HG23	1:C:2266:LEU:CD1	1.97	0.94
2:H:68:GLU:O	2:H:72:MSE:HB2	1.68	0.94
1:G:2129:LEU:O	1:G:2129:LEU:CD1	2.16	0.93
1:E:1996:VAL:HG22	1:E:2052:TRP:CE3	2.04	0.93
2:H:44:PRO:HG2	2:H:49:LEU:CD1	1.99	0.93
1:E:2135:ASN:HD21	1:E:2138:GLN:H	1.08	0.93
1:A:2020:MSE:HE1	1:A:2119:LEU:CB	1.99	0.92
1:G:2149:THR:O	1:G:2153:THR:HG22	1.68	0.92
1:A:2177:ARG:HB3	1:A:2180:ASN:ND2	1.84	0.92
1:A:2014:GLN:NE2	1:A:2018:GLN:HG3	1.85	0.92
1:C:2313:LEU:HD21	1:E:2347:VAL:HG11	1.49	0.92
1:E:2135:ASN:HD21	1:E:2138:GLN:N	1.67	0.92
1:A:1996:VAL:HG21	1:A:2052:TRP:CZ3	2.05	0.91
1:E:2326:ILE:HD11	1:E:2346:LEU:HB2	0.94	0.91
2:B:44:PRO:CG	2:B:49:LEU:CD1	2.48	0.91
1:C:2231:VAL:HG11	1:C:2266:LEU:CD2	2.01	0.91
2:H:89:ALA:O	2:H:92:VAL:HG22	1.69	0.91
2:B:91:ARG:HG3	2:B:139:TYR:HE2	1.33	0.91
1:E:2235:PHE:CD2	1:E:2241:GLU:HG2	2.06	0.91
2:D:141:GLU:O	2:D:145:MSE:HB3	1.70	0.90
1:A:2131:LEU:HD11	1:A:2138:GLN:HB3	1.52	0.90
2:H:82:SER:O	2:H:86:ILE:HG13	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2362:ILE:CG2	1:A:2370:TRP:CE3	2.55	0.89
1:E:2233:VAL:HG12	1:E:2234:ARG:H	1.36	0.89
1:E:2135:ASN:ND2	1:E:2138:GLN:H	1.69	0.89
2:B:138:ASN:HB3	2:B:141:GLU:HB2	1.55	0.89
1:C:2329:PHE:HD2	1:C:2362:ILE:HD11	1.33	0.89
1:G:2269:ILE:HD13	2:H:113:LEU:CD1	2.01	0.89
1:A:2210:SER:HA	1:A:2213:LYS:HE3	1.54	0.89
1:C:2128:GLY:HA2	1:C:2131:LEU:HB3	1.56	0.88
1:E:2004:VAL:HG12	1:E:2144:SER:HB2	1.55	0.88
1:E:2004:VAL:HG12	1:E:2144:SER:HA	1.55	0.88
2:B:20:PHE:CD1	2:B:36:VAL:HG22	2.08	0.88
1:G:2352:LEU:HD13	1:G:2358:ARG:HD2	1.54	0.88
1:E:2358:ARG:HD3	1:E:2358:ARG:N	1.89	0.88
1:C:2264:VAL:HG11	2:D:92:VAL:CG2	2.03	0.88
2:B:73:MSE:O	2:B:77:MSE:HB2	1.74	0.88
2:B:99:GLY:O	2:B:139:TYR:CD1	2.26	0.87
1:C:2231:VAL:CG1	1:C:2266:LEU:HD22	2.03	0.87
2:F:44:PRO:HG2	2:F:49:LEU:HD11	1.57	0.87
2:B:52:MSE:HE2	2:B:72:MSE:CB	2.05	0.87
1:A:2242:ARG:HH11	1:A:2242:ARG:HB2	1.39	0.86
1:E:2358:ARG:HH21	1:E:2358:ARG:H	1.22	0.86
2:H:30:THR:HA	2:H:33:LEU:HD23	1.56	0.86
1:C:2231:VAL:HG11	1:C:2266:LEU:HD22	1.54	0.85
1:G:2129:LEU:HD13	1:G:2129:LEU:C	2.02	0.85
1:A:2362:ILE:CG2	1:A:2370:TRP:CD2	2.60	0.85
1:A:2014:GLN:HE21	1:A:2018:GLN:CD	1.85	0.84
2:B:37:MSE:HG2	2:B:73:MSE:HE1	1.57	0.84
2:B:91:ARG:CG	2:B:139:TYR:CE2	2.59	0.84
1:E:2264:VAL:HG11	2:F:92:VAL:HG21	1.60	0.84
2:D:30:THR:HG22	2:D:64:ILE:HG13	1.58	0.83
1:A:2032:PRO:HB2	1:A:2035:GLN:HG2	1.57	0.83
1:E:2051:ASP:HB3	1:E:2054:LYS:HB2	1.60	0.83
2:F:44:PRO:HB2	2:F:49:LEU:HD12	1.60	0.83
1:E:2216:PRO:HD2	1:E:2219:GLN:HG3	1.59	0.83
1:A:2029:ASN:ND2	1:A:2115:PHE:HE1	1.75	0.83
1:C:2272:MSE:HE2	2:D:86:ILE:CG2	2.09	0.83
1:E:2020:MSE:HE1	1:E:2119:LEU:O	1.79	0.83
1:A:2020:MSE:HE3	1:A:2119:LEU:HG	1.61	0.83
1:A:2177:ARG:HB3	1:A:2180:ASN:HD22	1.42	0.82
2:B:56:VAL:HG21	2:B:68:GLU:CG	2.08	0.82
2:D:52:MSE:HB3	2:D:72:MSE:SE	2.30	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2177:ARG:HB2	1:E:2180:ASN:HD22	1.41	0.82
1:G:2264:VAL:HG11	2:H:92:VAL:CG1	2.09	0.82
1:G:2349:ASN:HB3	1:G:2364:GLN:HB2	1.62	0.82
1:G:2016:MSE:HE2	1:G:2145:ILE:HD11	1.62	0.81
1:E:2132:ASP:N	1:E:2138:GLN:HE21	1.76	0.81
2:B:52:MSE:O	2:B:56:VAL:CG1	2.28	0.81
1:C:2006:VAL:HG21	1:C:2140:GLN:HG2	1.61	0.81
2:B:91:ARG:HG3	2:B:139:TYR:CE2	2.14	0.81
2:F:29:THR:O	2:F:30:THR:HG22	1.80	0.81
1:E:2358:ARG:HD3	1:E:2358:ARG:H	1.44	0.81
2:F:73:MSE:O	2:F:77:MSE:HG3	1.81	0.81
2:H:37:MSE:CE	2:H:44:PRO:HG3	2.11	0.81
2:B:69:PHE:CZ	2:B:73:MSE:CE	2.62	0.80
1:A:2242:ARG:HB2	1:A:2242:ARG:NH1	1.96	0.80
2:B:44:PRO:HB2	2:B:49:LEU:HD13	1.63	0.80
1:A:1996:VAL:CG2	1:A:2052:TRP:CZ3	2.62	0.80
1:A:2020:MSE:CE	1:A:2119:LEU:CB	2.56	0.80
1:G:2129:LEU:HD12	1:G:2130:PHE:CZ	2.16	0.79
1:E:2314:LEU:CD2	1:E:2326:ILE:HD12	2.12	0.79
2:B:44:PRO:HG2	2:B:49:LEU:HD11	1.65	0.79
2:B:91:ARG:HG2	2:B:139:TYR:OH	1.82	0.79
1:C:2343:GLU:OE2	1:E:2358:ARG:HG2	1.82	0.79
1:A:2362:ILE:HG21	1:A:2370:TRP:CD2	2.18	0.79
2:B:44:PRO:HB2	2:B:49:LEU:CD1	2.13	0.79
1:E:2250:ASN:CB	1:E:2251:PRO:HD3	2.12	0.79
1:A:2029:ASN:HD22	1:A:2115:PHE:HE1	1.29	0.78
1:C:2010:ASP:O	1:C:2014:GLN:HG2	1.83	0.78
1:A:2131:LEU:HD12	1:A:2132:ASP:H	1.46	0.78
1:E:2360:ARG:NH1	1:E:2363:ALA:HB2	1.98	0.78
2:B:69:PHE:CE1	2:B:73:MSE:CE	2.66	0.78
1:G:2129:LEU:HD12	1:G:2130:PHE:CD1	2.19	0.78
1:A:2032:PRO:HG2	1:A:2035:GLN:HG3	1.63	0.78
2:B:44:PRO:HG3	2:B:49:LEU:HD11	1.64	0.78
1:E:2024:ILE:HD13	1:E:2039:LEU:HD23	1.66	0.78
1:C:2014:GLN:O	1:C:2018:GLN:HG2	1.85	0.77
1:G:2052:TRP:O	1:G:2056:VAL:HG23	1.84	0.77
2:D:117:LEU:HD23	2:D:122:VAL:HG22	1.66	0.77
1:E:2004:VAL:HG12	1:E:2144:SER:CB	2.14	0.77
2:H:52:MSE:CG	2:H:72:MSE:SE	2.83	0.77
1:A:2014:GLN:NE2	1:A:2018:GLN:CD	2.43	0.77
2:H:44:PRO:HG2	2:H:49:LEU:HD11	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:10:ILE:CG2	2:H:70:LEU:HD11	2.13	0.76
2:B:37:MSE:HG2	2:B:73:MSE:HE2	1.66	0.76
1:E:2193:LEU:HB3	1:E:2199:VAL:CG2	2.14	0.76
2:B:44:PRO:HG2	2:B:49:LEU:CD1	2.14	0.76
1:E:2264:VAL:HG11	2:F:92:VAL:CG2	2.15	0.76
1:G:2268:ALA:HB1	2:H:86:ILE:HG12	1.67	0.76
2:B:91:ARG:HG2	2:B:139:TYR:CE2	2.19	0.76
2:F:33:LEU:O	2:F:37:MSE:HG3	1.86	0.76
2:B:56:VAL:CG2	2:B:68:GLU:HG2	2.14	0.76
2:B:138:ASN:ND2	2:B:141:GLU:HG3	1.94	0.76
2:D:10:ILE:CG1	2:D:70:LEU:HD11	2.14	0.76
1:G:1970:VAL:HG11	1:G:2069:PHE:CD1	2.21	0.76
2:H:69:PHE:CE2	2:H:73:MSE:CE	2.69	0.76
1:A:2365:LYS:C	1:A:2366:GLU:OE1	2.29	0.75
1:E:2004:VAL:HG11	1:E:2144:SER:HA	1.67	0.75
1:G:2352:LEU:HD13	1:G:2358:ARG:CD	2.16	0.75
1:A:2014:GLN:NE2	1:A:2018:GLN:CG	2.49	0.75
1:C:2182:PHE:HA	1:C:2186:GLU:HB2	1.65	0.75
2:B:20:PHE:CE1	2:B:36:VAL:HG22	2.20	0.75
2:D:50:GLN:NE2	2:D:50:GLN:HA	2.02	0.75
1:E:2250:ASN:HB3	1:E:2251:PRO:CD	2.15	0.75
1:G:2207:LYS:HB3	1:G:2208:PRO:HD2	1.66	0.75
1:C:2313:LEU:CD2	1:E:2347:VAL:HG11	2.16	0.75
2:F:6:THR:HG22	2:F:8:GLU:HG3	1.67	0.75
2:F:81:ASP:O	2:F:85:GLU:HG3	1.86	0.75
1:E:2359:THR:HG21	4:E:2406:HOH:O	1.87	0.75
1:E:2362:ILE:CG2	1:E:2370:TRP:CE3	2.69	0.75
1:G:2269:ILE:HD13	2:H:113:LEU:HD13	1.67	0.75
1:A:2250:ASN:HB2	1:A:2251:PRO:HD3	0.78	0.74
2:H:37:MSE:HE2	2:H:44:PRO:HG3	1.68	0.74
1:G:2131:LEU:N	1:G:2131:LEU:HD13	2.02	0.74
1:G:2295:GLU:HA	1:G:2295:GLU:OE1	1.86	0.74
1:A:2294:GLU:OE2	1:A:2294:GLU:HA	1.87	0.74
1:E:2213:LYS:O	1:E:2215:LEU:CD2	2.35	0.74
1:C:2196:GLU:HB2	1:C:2198:LEU:HD12	1.70	0.74
2:D:66:PHE:N	2:D:67:PRO:HD2	2.03	0.74
1:E:2004:VAL:HG12	1:E:2144:SER:CA	2.18	0.74
1:C:2290:VAL:HG22	1:C:2299:VAL:HG22	1.70	0.74
1:A:2029:ASN:ND2	1:A:2115:PHE:CE1	2.55	0.74
2:B:37:MSE:HA	2:B:73:MSE:HE1	1.70	0.74
1:A:2298:GLU:HB3	1:A:2300:ARG:NH1	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2074:ALA:O	1:C:2075:GLU:HG2	1.88	0.73
2:H:96:ASP:OD1	2:H:96:ASP:N	2.15	0.73
1:E:2233:VAL:HG12	1:E:2234:ARG:N	2.02	0.73
1:A:2245:GLU:HA	1:A:2245:GLU:OE2	1.85	0.73
1:G:2094:LEU:O	1:G:2098:GLN:HG2	1.88	0.73
1:G:2328:ARG:HH21	2:H:40:LEU:HD23	1.53	0.73
2:F:30:THR:HA	2:F:33:LEU:HD23	1.70	0.73
1:G:2269:ILE:HD13	2:H:113:LEU:HD12	1.70	0.73
1:E:2224:LEU:O	1:E:2229:VAL:HG11	1.89	0.73
2:F:52:MSE:CB	2:F:72:MSE:SE	2.87	0.73
2:H:88:GLU:O	2:H:92:VAL:HG13	1.89	0.72
1:A:2362:ILE:HG21	1:A:2370:TRP:CE3	2.25	0.72
2:H:30:THR:HB	2:H:64:ILE:HG13	1.70	0.72
1:A:2354:HIS:CD2	1:A:2358:ARG:HB2	2.23	0.72
2:B:99:GLY:O	2:B:139:TYR:CE1	2.43	0.72
1:E:2006:VAL:HG11	1:E:2141:LEU:HD23	1.72	0.72
2:B:44:PRO:CB	2:B:49:LEU:CD1	2.66	0.72
2:B:105:GLU:O	2:B:109:VAL:HG23	1.88	0.72
1:E:2232:LYS:HE3	4:E:2402:HOH:O	1.89	0.72
1:A:2210:SER:CA	1:A:2213:LYS:HE3	2.20	0.72
1:E:2283:ARG:HG2	1:E:2288:LEU:O	1.90	0.72
2:F:88:GLU:O	2:F:92:VAL:HG23	1.90	0.72
1:A:2172:ALA:O	1:A:2206:ASP:HA	1.90	0.71
1:E:1970:VAL:HG11	1:E:2069:PHE:CD1	2.25	0.71
2:H:10:ILE:HD13	2:H:70:LEU:HD21	1.72	0.71
2:F:44:PRO:HB2	2:F:49:LEU:CD1	2.19	0.71
1:C:2224:LEU:HD12	1:C:2224:LEU:N	2.05	0.71
2:H:30:THR:HB	2:H:64:ILE:CG1	2.19	0.71
2:H:124:GLN:O	2:H:128:GLU:HG2	1.90	0.71
2:B:52:MSE:HB2	2:B:72:MSE:SE	2.40	0.71
1:G:1983:TRP:HA	1:G:1986:THR:CG2	2.21	0.71
1:E:2223:ARG:CZ	2:F:115:GLU:OE2	2.39	0.71
2:H:42:GLN:NE2	2:H:76:LYS:HG3	2.05	0.71
2:D:45:THR:HG23	2:D:48:GLU:H	1.56	0.71
2:D:6:THR:HG22	2:D:9:GLN:H	1.53	0.70
1:A:2250:ASN:O	1:E:2026:HIS:HB3	1.91	0.70
1:E:2172:ALA:O	1:E:2206:ASP:HA	1.91	0.70
1:A:2014:GLN:HE21	1:A:2018:GLN:CG	2.04	0.70
1:E:1994:LYS:HE2	1:E:2053:ASP:HB2	1.74	0.70
2:D:90:PHE:HZ	2:D:110:MSE:HE3	1.55	0.70
1:A:2033:LYS:H	1:A:2033:LYS:CD	1.93	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1996:VAL:CG2	1:E:2052:TRP:CE3	2.75	0.70
2:H:30:THR:CA	2:H:33:LEU:HD23	2.21	0.70
2:B:52:MSE:CB	2:B:72:MSE:SE	2.90	0.70
2:F:44:PRO:CG	2:F:49:LEU:HD11	2.22	0.70
1:A:2020:MSE:HE1	1:A:2119:LEU:CA	2.22	0.69
1:C:2006:VAL:CG1	1:C:2144:SER:HB2	2.22	0.69
1:E:2234:ARG:HA	1:E:2258:THR:O	1.91	0.69
1:E:2308:LYS:O	1:E:2337:PHE:HZ	1.75	0.69
1:A:2329:PHE:HA	2:B:19:LEU:HD23	1.73	0.69
1:E:2235:PHE:CE1	1:E:2254:TYR:CD1	2.80	0.69
2:H:44:PRO:HB3	2:H:76:LYS:HE2	1.75	0.69
1:C:2205:LEU:HA	1:C:2212:TYR:OH	1.93	0.69
2:H:33:LEU:C	2:H:33:LEU:HD12	2.17	0.69
2:D:131:ILE:HG12	2:D:141:GLU:OE1	1.92	0.69
1:E:2032:PRO:HB2	1:E:2035:GLN:CB	2.22	0.69
1:C:2195:ARG:HH22	2:D:111:THR:HG23	1.58	0.69
1:E:2087:PHE:HE1	1:E:2088:LYS:HE2	1.57	0.69
2:B:33:LEU:HD11	2:B:69:PHE:HD1	1.58	0.68
2:H:83:GLU:O	2:H:87:ARG:HG2	1.93	0.68
2:H:20:PHE:HB2	2:H:28:ILE:CD1	2.22	0.68
1:G:2006:VAL:HG13	1:G:2144:SER:HB3	1.74	0.68
1:G:2177:ARG:HB3	1:G:2180:ASN:HD22	1.58	0.68
1:E:2141:LEU:HD13	1:E:2141:LEU:O	1.93	0.68
1:A:1996:VAL:HG22	1:A:2052:TRP:HE3	1.53	0.68
1:A:2169:TYR:CE1	1:A:2203:ARG:HD3	2.28	0.68
1:E:2087:PHE:CE1	1:E:2088:LYS:HE2	2.28	0.68
1:A:2224:LEU:H	1:A:2224:LEU:CD1	2.07	0.68
2:B:91:ARG:O	2:B:94:ASP:HB2	1.94	0.68
1:C:2120:ASN:ND2	1:C:2152:ASN:HD22	1.91	0.68
1:E:2141:LEU:HD13	1:E:2141:LEU:C	2.18	0.68
1:G:2352:LEU:HD13	1:G:2358:ARG:CG	2.24	0.68
1:C:2006:VAL:HG22	1:C:2006:VAL:O	1.93	0.68
1:A:2032:PRO:CB	1:A:2035:GLN:CG	2.50	0.67
2:B:91:ARG:HG2	2:B:139:TYR:CZ	2.29	0.67
1:A:2131:LEU:CD1	1:A:2138:GLN:HB3	2.23	0.67
1:A:2352:LEU:HD23	1:A:2360:ARG:HA	1.74	0.67
1:A:2362:ILE:HG22	1:A:2370:TRP:HA	1.75	0.67
1:E:2324:LYS:O	1:E:2328:ARG:HG3	1.95	0.67
1:A:2129:LEU:HD12	1:E:2256:ALA:HB2	1.76	0.67
2:H:66:PHE:CZ	2:H:70:LEU:HD13	2.29	0.67
2:D:37:MSE:CE	2:D:73:MSE:HE2	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2016:MSE:HE1	1:E:2145:ILE:HD11	1.75	0.67
1:G:2290:VAL:HG22	1:G:2299:VAL:CG2	2.24	0.67
1:E:2004:VAL:CG1	1:E:2144:SER:CA	2.70	0.67
1:E:2016:MSE:CE	1:E:2145:ILE:CD1	2.73	0.67
1:E:2034:ASP:OD1	1:E:2035:GLN:N	2.28	0.67
1:E:2226:ASP:O	1:E:2229:VAL:HG12	1.95	0.67
2:B:132:ASP:HB2	2:B:134:ASP:OD1	1.95	0.66
1:E:2126:TRP:CD1	1:E:2130:PHE:HE1	2.13	0.66
1:A:2224:LEU:HD12	1:A:2224:LEU:N	2.10	0.66
2:F:30:THR:HB	2:F:62:GLY:HA2	1.76	0.66
2:F:105:GLU:O	2:F:109:VAL:HG23	1.96	0.66
1:A:2210:SER:HA	1:A:2213:LYS:CE	2.25	0.66
1:A:2362:ILE:HG23	1:A:2370:TRP:CE3	2.29	0.66
2:B:69:PHE:CE1	2:B:73:MSE:HE2	2.29	0.66
1:C:2231:VAL:HG11	1:C:2266:LEU:CD1	2.25	0.66
2:H:6:THR:HG22	2:H:7:GLU:N	2.09	0.66
1:E:2214:ASP:C	1:E:2215:LEU:HD22	2.20	0.66
1:E:2177:ARG:CB	1:E:2180:ASN:ND2	2.53	0.66
1:C:2313:LEU:HD21	1:E:2347:VAL:CG1	2.25	0.66
2:D:25:ASP:HA	2:H:61:ASN:HB2	1.78	0.66
2:D:90:PHE:CZ	2:D:110:MSE:HE3	2.29	0.66
2:B:66:PHE:N	2:B:67:PRO:HD2	2.11	0.66
1:C:2224:LEU:HD12	1:C:2224:LEU:H	1.58	0.66
2:H:63:THR:HG22	2:H:63:THR:O	1.95	0.66
2:B:90:PHE:HB3	2:B:139:TYR:HD2	1.60	0.65
1:G:1983:TRP:HA	1:G:1986:THR:HG23	1.76	0.65
2:B:61:ASN:OD1	2:B:61:ASN:O	2.14	0.65
2:D:37:MSE:HE3	2:D:73:MSE:CE	2.21	0.65
1:G:1983:TRP:CA	1:G:1986:THR:HG23	2.27	0.65
1:G:1983:TRP:C	1:G:1986:THR:HG23	2.22	0.65
1:G:2054:LYS:HE2	4:G:2402:HOH:O	1.96	0.65
1:A:2193:LEU:HB3	1:A:2199:VAL:HG23	1.79	0.65
2:B:129:ALA:HB2	2:B:142:PHE:HD1	1.62	0.65
1:E:2016:MSE:CE	1:E:2145:ILE:HD11	2.27	0.65
1:A:2210:SER:CB	1:A:2213:LYS:HE3	2.27	0.65
1:A:2217:ALA:HA	1:A:2220:ILE:HD12	1.76	0.65
1:E:2126:TRP:CD1	1:E:2130:PHE:CE1	2.85	0.65
1:E:2365:LYS:O	1:E:2366:GLU:CG	2.41	0.65
1:A:2132:ASP:OD1	1:A:2133:PRO:HD2	1.96	0.65
2:B:33:LEU:HD11	2:B:69:PHE:CD1	2.32	0.65
1:C:2264:VAL:HG23	1:C:2266:LEU:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2299:VAL:HG21	1:C:2312:ILE:CD1	2.27	0.65
2:B:44:PRO:CB	2:B:49:LEU:HD13	2.26	0.64
1:A:2242:ARG:HH11	1:A:2242:ARG:CB	2.09	0.64
2:B:138:ASN:HD22	2:B:141:GLU:CG	1.99	0.64
2:F:122:VAL:O	2:F:126:ILE:HG12	1.98	0.64
2:B:125:MSE:HG3	2:B:126:ILE:HD13	1.79	0.64
1:C:1982:ARG:O	1:C:1986:THR:HG23	1.97	0.64
1:G:2006:VAL:CG1	1:G:2140:GLN:HE21	2.11	0.64
2:B:33:LEU:CD1	2:B:69:PHE:CD1	2.81	0.64
2:F:132:ASP:OD1	2:F:132:ASP:N	2.31	0.64
1:G:2138:GLN:N	1:G:2138:GLN:OE1	2.31	0.64
2:H:44:PRO:HB3	2:H:76:LYS:HZ3	1.62	0.64
1:A:2158:SER:O	1:A:2162:THR:HG23	1.98	0.64
2:B:117:LEU:HD23	2:B:122:VAL:HG22	1.79	0.64
1:G:2310:LYS:NZ	1:G:2340:MSE:O	2.31	0.64
1:A:2129:LEU:CD1	1:E:2256:ALA:HB2	2.28	0.64
1:E:2016:MSE:HE1	1:E:2145:ILE:CD1	2.28	0.64
2:D:124:GLN:O	2:D:128:GLU:HG3	1.98	0.63
2:H:6:THR:HG22	2:H:8:GLU:OE1	1.97	0.63
1:A:2308:LYS:NZ	1:A:2338:GLU:OE1	2.25	0.63
2:B:100:TYR:CE2	2:B:138:ASN:HB2	2.34	0.63
2:D:101:ILE:HG12	2:D:139:TYR:HD1	1.63	0.63
1:E:2131:LEU:HD21	1:E:2141:LEU:HD12	1.79	0.63
2:B:128:GLU:HB3	2:B:145:MSE:HE1	1.81	0.63
1:C:2233:VAL:HG23	1:C:2262:LEU:CD1	2.28	0.63
1:A:2354:HIS:NE2	1:A:2358:ARG:HB2	2.13	0.63
1:E:2004:VAL:CG1	1:E:2144:SER:CB	2.77	0.63
2:B:126:ILE:HD13	2:B:126:ILE:N	2.14	0.63
1:C:2205:LEU:HG	1:C:2212:TYR:CZ	2.33	0.63
2:D:129:ALA:HB2	2:D:142:PHE:CD1	2.34	0.63
2:B:52:MSE:CE	2:B:72:MSE:HB3	2.21	0.63
1:A:2037:GLU:O	1:A:2041:THR:HG23	1.99	0.62
1:A:2040:ALA:O	1:A:2044:VAL:HG23	1.99	0.62
1:C:2120:ASN:HD21	1:C:2152:ASN:HD22	1.46	0.62
1:C:2006:VAL:HG21	1:C:2140:GLN:CG	2.29	0.62
1:E:2308:LYS:O	1:E:2337:PHE:CZ	2.52	0.62
2:H:6:THR:CG2	2:H:8:GLU:OE1	2.47	0.62
1:C:2001:PHE:HE2	1:C:2150:PHE:HD1	1.45	0.62
2:B:100:TYR:HD2	2:B:137:VAL:C	2.07	0.62
2:D:30:THR:CG2	2:D:64:ILE:HG12	2.23	0.62
4:E:2401:HOH:O	2:F:111:THR:HG21	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:TYR:HD2	2:B:138:ASN:N	1.97	0.62
1:E:1994:LYS:HE2	1:E:2053:ASP:CB	2.30	0.62
2:H:91:ARG:HG2	2:H:139:TYR:OH	2.00	0.61
1:C:2231:VAL:HG12	1:C:2266:LEU:HD22	1.80	0.61
1:E:1987:ASP:OD2	2:F:126:ILE:HG21	1.99	0.61
1:E:2013:LYS:O	1:E:2017:ILE:CG1	2.46	0.61
1:C:2370:TRP:NE1	2:D:22:LYS:HG2	2.15	0.61
2:F:66:PHE:N	2:F:67:PRO:HD2	2.15	0.61
1:E:2004:VAL:CG1	1:E:2144:SER:HB2	2.29	0.61
2:H:44:PRO:HB3	2:H:76:LYS:CE	2.30	0.61
2:H:83:GLU:O	2:H:87:ARG:CG	2.48	0.61
1:G:2174:GLY:O	1:G:2230:ALA:HB3	2.00	0.61
1:C:2224:LEU:H	1:C:2224:LEU:CD1	2.13	0.61
1:E:2233:VAL:CG1	1:E:2234:ARG:H	2.09	0.61
1:E:2245:GLU:OE1	1:E:2245:GLU:HA	2.01	0.61
2:D:96:ASP:OD2	2:D:96:ASP:N	2.34	0.61
1:E:2034:ASP:OD1	1:E:2035:GLN:HG2	2.01	0.61
1:A:2002:GLU:O	1:A:2002:GLU:HG3	2.00	0.60
1:A:2020:MSE:CE	1:A:2119:LEU:HG	2.31	0.60
1:A:2098:GLN:NE2	1:A:2217:ALA:HB1	2.15	0.60
1:E:2008:VAL:HG12	1:E:2009:SER:N	2.15	0.60
1:G:2006:VAL:HB	1:G:2140:GLN:NE2	2.16	0.60
1:E:2214:ASP:O	1:E:2215:LEU:HD22	2.02	0.60
1:A:2020:MSE:HE3	1:A:2119:LEU:CG	2.32	0.60
1:A:2324:LYS:O	1:A:2328:ARG:HG3	2.02	0.60
1:E:2082:TRP:HA	1:E:2171:ILE:HB	1.84	0.60
1:G:2098:GLN:HE22	1:G:2217:ALA:HB1	1.66	0.60
1:G:2315:ASP:HB3	1:G:2322:GLN:HE22	1.67	0.60
1:G:2352:LEU:HD13	1:G:2358:ARG:HG3	1.83	0.60
2:H:91:ARG:CG	2:H:139:TYR:OH	2.49	0.60
1:E:2362:ILE:HG21	1:E:2370:TRP:CE3	2.36	0.60
1:G:2345:PHE:O	1:G:2351:VAL:HA	2.01	0.60
1:G:2349:ASN:HA	1:G:2364:GLN:OE1	2.01	0.60
2:B:6:THR:OG1	2:B:9:GLN:HG3	2.01	0.60
2:H:44:PRO:CG	2:H:49:LEU:CD1	2.77	0.60
2:H:98:ASN:H	2:H:98:ASN:ND2	1.99	0.60
1:A:1984:LEU:HA	2:B:107:ARG:HD3	1.82	0.60
1:A:2224:LEU:H	1:A:2224:LEU:HD12	1.62	0.60
1:C:2233:VAL:HG12	1:C:2234:ARG:N	2.15	0.60
1:G:2299:VAL:HG21	1:G:2312:ILE:CD1	2.32	0.60
2:H:33:LEU:HD12	2:H:34:GLY:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2016:MSE:CE	1:C:2141:LEU:HD11	2.31	0.60
1:A:2288:LEU:CD2	1:A:2337:PHE:HB2	2.32	0.60
1:E:2235:PHE:CZ	1:E:2254:TYR:CD1	2.90	0.60
2:H:27:THR:HG22	2:H:65:ASP:HB3	1.82	0.60
2:B:120:GLU:HB2	4:B:201:HOH:O	2.01	0.59
2:D:71:THR:O	2:D:74:ALA:HB3	2.02	0.59
1:G:2233:VAL:HG12	1:G:2234:ARG:N	2.17	0.59
1:E:2240:HIS:HA	1:E:2243:GLN:HG2	1.83	0.59
2:D:34:GLY:O	2:D:38:ARG:HB2	2.02	0.59
1:E:2051:ASP:CG	1:E:2054:LYS:HG3	2.26	0.59
1:C:2272:MSE:CE	2:D:86:ILE:CG2	2.80	0.59
1:C:2343:GLU:OE1	1:E:2358:ARG:CG	2.46	0.59
1:E:2017:ILE:HG12	1:E:2044:VAL:HG21	1.85	0.59
1:G:2315:ASP:N	1:G:2322:GLN:HE22	1.99	0.59
1:G:2352:LEU:CD1	1:G:2358:ARG:HD2	2.32	0.59
1:A:2298:GLU:CB	1:A:2300:ARG:NH1	2.66	0.59
1:A:2348:ASP:O	1:A:2350:LYS:HE2	2.03	0.59
1:A:2131:LEU:HD12	1:A:2132:ASP:N	2.17	0.59
1:A:2042:LEU:HD22	1:A:2061:LYS:HE3	1.84	0.59
1:A:2269:ILE:CD1	2:B:90:PHE:CZ	2.86	0.59
2:B:129:ALA:HB2	2:B:142:PHE:CD1	2.37	0.59
1:A:2250:ASN:CB	1:A:2251:PRO:CD	2.48	0.58
1:C:1973:ARG:HH12	1:C:2070:GLU:HG2	1.67	0.58
1:C:2324:LYS:O	1:C:2328:ARG:HG3	2.02	0.58
1:E:1970:VAL:HG12	1:E:2069:PHE:HB2	1.85	0.58
1:G:2005:ASP:OD1	1:G:2050:TYR:CE2	2.55	0.58
1:E:2012:VAL:HA	1:E:2015:ARG:HD3	1.84	0.58
2:D:139:TYR:HD2	2:D:139:TYR:O	1.85	0.58
1:E:2032:PRO:CB	1:E:2035:GLN:HB2	2.27	0.58
1:E:2207:LYS:HB3	1:E:2208:PRO:HD2	1.84	0.58
1:E:2235:PHE:CZ	1:E:2254:TYR:HD1	2.21	0.58
2:B:44:PRO:CG	2:B:49:LEU:HD13	2.33	0.58
1:A:2138:GLN:HA	1:A:2138:GLN:NE2	2.18	0.58
1:E:2213:LYS:O	1:E:2215:LEU:HD22	2.02	0.58
1:C:2265:LYS:O	1:C:2266:LEU:HB2	2.03	0.58
1:C:2360:ARG:NH1	1:C:2371:THR:O	2.36	0.58
2:D:42:GLN:HE21	2:D:76:LYS:HE3	1.68	0.58
2:F:56:VAL:O	2:F:56:VAL:HG13	2.04	0.58
1:C:2314:LEU:HD13	1:C:2322:GLN:HG2	1.85	0.58
1:E:2132:ASP:CG	1:E:2132:ASP:O	2.45	0.58
1:E:2177:ARG:CB	1:E:2180:ASN:HD22	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:PRO:HB3	2:H:76:LYS:NZ	2.18	0.58
1:A:2358:ARG:O	1:A:2358:ARG:NE	2.37	0.57
1:G:2345:PHE:HB2	1:G:2352:LEU:HG	1.85	0.57
1:A:2286:ARG:NH2	1:A:2331:LEU:O	2.36	0.57
2:B:87:ARG:HD3	2:B:140:GLU:CG	2.33	0.57
1:G:2352:LEU:CD1	1:G:2358:ARG:HG3	2.34	0.57
1:A:2014:GLN:HE21	1:A:2018:GLN:HG3	1.63	0.57
1:E:2223:ARG:NE	2:F:115:GLU:OE2	2.37	0.57
2:F:118:THR:HB	2:F:121:GLU:HB2	1.85	0.57
2:H:69:PHE:HD2	2:H:69:PHE:O	1.88	0.57
2:D:5:LEU:HD12	2:D:5:LEU:N	2.19	0.57
1:G:2004:VAL:O	1:G:2004:VAL:HG12	2.05	0.57
1:G:2280:TYR:O	1:G:2283:ARG:HB2	2.04	0.57
2:F:52:MSE:CG	2:F:72:MSE:SE	3.02	0.57
2:H:69:PHE:C	2:H:69:PHE:CD2	2.82	0.57
1:C:2328:ARG:NH2	2:D:40:LEU:HD23	2.19	0.57
1:E:2288:LEU:CD2	1:E:2337:PHE:HB2	2.35	0.57
1:A:2266:LEU:HG	2:B:113:LEU:HD11	1.87	0.57
1:G:2129:LEU:CD1	1:G:2129:LEU:C	2.71	0.57
1:A:2175:GLY:HA3	1:A:2230:ALA:O	2.05	0.57
1:A:2299:VAL:HG21	1:A:2312:ILE:CD1	2.34	0.57
1:C:2231:VAL:HG11	1:C:2266:LEU:HD13	1.86	0.57
2:H:42:GLN:HE21	2:H:76:LYS:HG3	1.70	0.57
1:C:2212:TYR:CD1	1:C:2220:ILE:HG23	2.39	0.57
1:C:2139:ASN:ND2	1:C:2139:ASN:H	2.01	0.56
2:F:25:ASP:OD1	2:F:25:ASP:N	2.31	0.56
1:A:2292:GLU:HG2	1:A:2297:PHE:CE1	2.40	0.56
1:C:2330:ILE:HG12	1:C:2340:MSE:HE3	1.85	0.56
1:E:2326:ILE:HG13	1:E:2346:LEU:HD22	1.86	0.56
1:E:2362:ILE:HG22	1:E:2370:TRP:HA	1.86	0.56
1:C:2177:ARG:HB3	1:C:2180:ASN:ND2	2.20	0.56
1:C:2299:VAL:CG2	1:C:2312:ILE:CD1	2.83	0.56
2:D:118:THR:OG1	2:D:121:GLU:HG3	2.05	0.56
1:E:2006:VAL:CG1	1:E:2141:LEU:HD23	2.35	0.56
1:E:2008:VAL:CG1	1:E:2012:VAL:HB	2.35	0.56
1:E:2177:ARG:HB2	1:E:2180:ASN:HD21	1.66	0.56
1:E:2237:ALA:O	1:E:2241:GLU:HG3	2.05	0.56
1:C:2234:ARG:NH2	1:C:2257:ASP:HB2	2.21	0.56
1:A:1994:LYS:O	1:A:2052:TRP:N	2.38	0.56
2:H:6:THR:HG22	2:H:8:GLU:H	1.70	0.56
2:B:33:LEU:CD1	2:B:69:PHE:HD1	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:PHE:O	2:B:72:MSE:HG3	2.05	0.56
1:G:2350:LYS:NZ	1:G:2363:ALA:HA	2.21	0.56
1:C:2196:GLU:CB	1:C:2198:LEU:HD12	2.35	0.56
2:H:107:ARG:NH2	2:H:123:ASP:HA	2.21	0.56
1:C:2089:GLN:HE21	1:C:2209:VAL:HG11	1.70	0.56
2:D:94:ASP:OD1	2:D:97:GLY:N	2.39	0.56
1:G:2329:PHE:CE1	1:G:2344:LEU:HD21	2.40	0.56
1:G:2341:PRO:HG2	1:G:2344:LEU:HD13	1.88	0.56
2:B:23:ASP:HB2	2:B:25:ASP:OD2	2.06	0.56
1:A:2362:ILE:HG22	1:A:2370:TRP:CD2	2.41	0.55
1:A:2294:GLU:O	1:A:2295:GLU:HG2	2.06	0.55
1:C:2016:MSE:HG2	1:C:2126:TRP:CH2	2.42	0.55
1:C:2269:ILE:HD12	2:D:110:MSE:HE1	1.87	0.55
1:E:2190:LEU:HB3	1:E:2202:ILE:HD11	1.88	0.55
2:F:73:MSE:O	2:F:77:MSE:CG	2.55	0.55
1:C:2205:LEU:HG	1:C:2212:TYR:CE2	2.42	0.55
1:C:2299:VAL:HG23	1:C:2312:ILE:HD12	1.88	0.55
1:E:2182:PHE:HA	1:E:2186:GLU:HB2	1.88	0.55
1:G:2095:ASP:OD1	1:G:2104:VAL:HG13	2.07	0.55
1:C:2006:VAL:HG12	1:C:2144:SER:HB2	1.89	0.55
2:F:48:GLU:CD	2:F:76:LYS:HZ3	2.15	0.55
2:B:20:PHE:CD1	2:B:36:VAL:CG2	2.87	0.55
2:D:37:MSE:CE	2:D:76:LYS:HG2	2.36	0.55
1:G:2131:LEU:N	1:G:2131:LEU:CD1	2.70	0.55
1:A:2157:SER:OG	1:A:2185:VAL:HG21	2.06	0.55
2:B:100:TYR:HA	2:B:137:VAL:O	2.07	0.55
2:D:136:GLN:HA	2:D:136:GLN:NE2	2.22	0.55
2:F:23:ASP:OD1	2:F:23:ASP:N	2.40	0.55
1:G:2016:MSE:HE3	1:G:2145:ILE:HD11	1.83	0.55
1:C:2172:ALA:HB3	1:C:2204:LEU:HD11	1.89	0.55
1:E:2354:HIS:CE1	1:E:2356:ASP:O	2.60	0.55
1:E:2085:LYS:O	1:E:2086:ASN:OD1	2.24	0.54
2:H:84:GLU:O	2:H:88:GLU:HG2	2.07	0.54
1:A:2051:ASP:CG	1:A:2054:LYS:HD2	2.33	0.54
1:A:2329:PHE:HD2	1:A:2362:ILE:HD11	1.73	0.54
2:D:145:MSE:O	2:D:148:ALA:O	2.25	0.54
2:H:89:ALA:O	2:H:92:VAL:CG2	2.49	0.54
1:C:2273:LEU:HD13	2:D:117:LEU:HD11	1.90	0.54
1:C:2280:TYR:O	1:C:2283:ARG:HB2	2.07	0.54
2:B:90:PHE:CB	2:B:139:TYR:HD2	2.20	0.54
1:C:2233:VAL:HG23	1:C:2262:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1973:ARG:NH1	1:E:2069:PHE:O	2.41	0.54
1:G:2182:PHE:HA	1:G:2186:GLU:HB2	1.88	0.54
1:A:2020:MSE:CE	1:A:2119:LEU:CG	2.85	0.54
2:B:69:PHE:HZ	2:B:73:MSE:HE3	1.62	0.54
2:B:100:TYR:CD2	2:B:138:ASN:N	2.76	0.54
1:A:2316:ASN:HB3	1:A:2322:GLN:HE21	1.73	0.54
1:C:2264:VAL:CG2	1:C:2266:LEU:CD1	2.79	0.54
1:G:2266:LEU:HD23	1:G:2266:LEU:O	2.08	0.54
2:F:125:MSE:CE	2:F:142:PHE:HZ	2.21	0.54
1:G:2021:SER:OG	1:G:2037:GLU:HA	2.07	0.54
1:A:1987:ASP:OD2	2:B:126:ILE:HG21	2.08	0.53
2:D:102:SER:HB2	2:D:105:GLU:HG3	1.90	0.53
1:E:2308:LYS:HD2	1:E:2308:LYS:C	2.33	0.53
2:B:128:GLU:OE1	2:B:145:MSE:HE1	2.07	0.53
2:F:64:ILE:HG23	2:F:64:ILE:O	2.09	0.53
2:H:6:THR:CG2	2:H:7:GLU:N	2.72	0.53
1:A:2231:VAL:HG22	1:A:2262:LEU:HB2	1.90	0.53
1:A:2235:PHE:HB2	1:A:2260:VAL:HG21	1.89	0.53
1:E:2224:LEU:N	1:E:2224:LEU:HD12	2.24	0.53
1:G:2302:TRP:CG	1:G:2303:PRO:HA	2.43	0.53
1:E:2250:ASN:CB	1:E:2251:PRO:CD	2.77	0.53
2:F:106:LEU:O	2:F:110:MSE:HG2	2.09	0.53
2:H:132:ASP:OD1	2:H:132:ASP:N	2.41	0.53
2:H:139:TYR:O	2:H:143:VAL:HG23	2.09	0.53
1:C:1973:ARG:NH1	1:C:2070:GLU:HG2	2.23	0.53
2:D:42:GLN:NE2	2:D:76:LYS:HE3	2.23	0.53
1:E:1978:ALA:O	1:E:1982:ARG:HG3	2.08	0.53
1:E:2016:MSE:CE	1:E:2145:ILE:HD13	2.37	0.53
1:E:2172:ALA:HB3	1:E:2204:LEU:HD11	1.90	0.53
2:F:50:GLN:OE1	2:F:50:GLN:HA	2.08	0.53
1:A:2333:ASN:HD21	1:A:2370:TRP:HZ3	1.55	0.53
2:B:37:MSE:CG	2:B:73:MSE:HE1	2.35	0.53
1:E:2046:SER:HB3	1:E:2054:LYS:HB3	1.90	0.53
1:C:2098:GLN:HE22	1:C:2217:ALA:HB1	1.74	0.53
2:D:141:GLU:O	2:D:145:MSE:HE3	2.09	0.53
2:F:45:THR:O	2:F:49:LEU:HD13	2.09	0.53
1:G:2212:TYR:HA	1:G:2215:LEU:HD12	1.90	0.53
2:B:13:PHE:N	2:B:13:PHE:CD1	2.77	0.53
1:C:2273:LEU:HD22	2:D:125:MSE:HE1	1.90	0.53
1:C:2299:VAL:CG2	1:C:2312:ILE:HD12	2.39	0.53
1:C:2351:VAL:HG21	1:C:2362:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2006:VAL:CG1	1:G:2144:SER:HB3	2.39	0.53
1:A:2168:VAL:O	1:A:2203:ARG:HG3	2.09	0.52
1:C:2233:VAL:HG12	1:C:2234:ARG:H	1.72	0.52
1:G:2083:SER:HB3	4:G:2403:HOH:O	2.08	0.52
2:F:44:PRO:CB	2:F:49:LEU:CD1	2.88	0.52
2:B:6:THR:HG23	2:B:9:GLN:CD	2.35	0.52
1:C:2137:GLU:CD	1:C:2140:GLN:OE1	2.53	0.52
1:E:2350:LYS:HD2	1:E:2360:ARG:CD	2.39	0.52
1:G:2020:MSE:HB3	1:G:2040:ALA:HB1	1.90	0.52
1:A:2014:GLN:HA	1:A:2017:ILE:HD12	1.92	0.52
1:A:2315:ASP:OD2	1:A:2322:GLN:NE2	2.42	0.52
1:C:2305:ILE:HG22	1:C:2305:ILE:O	2.08	0.52
1:C:2346:LEU:HD13	1:C:2351:VAL:HG23	1.92	0.52
1:C:2362:ILE:HD13	2:D:19:LEU:CD2	2.40	0.52
2:D:122:VAL:O	2:D:126:ILE:HG12	2.09	0.52
2:F:121:GLU:O	2:F:124:GLN:HG2	2.09	0.52
2:H:10:ILE:HG23	2:H:70:LEU:HD13	1.85	0.52
2:D:6:THR:HB	2:D:9:GLN:HG3	1.91	0.52
1:A:1991:ALA:HB2	1:A:1997:PRO:HD3	1.91	0.52
2:F:33:LEU:HD12	2:F:33:LEU:C	2.35	0.52
1:G:2006:VAL:HG11	1:G:2140:GLN:HE21	1.75	0.52
2:H:28:ILE:HG22	2:H:29:THR:N	2.25	0.52
1:A:2248:ALA:C	1:A:2250:ASN:H	2.18	0.52
1:C:2224:LEU:N	1:C:2224:LEU:CD1	2.71	0.52
2:D:37:MSE:HE1	2:D:76:LYS:HG2	1.91	0.52
2:F:63:THR:HG22	2:F:63:THR:O	2.10	0.52
2:H:20:PHE:C	2:H:28:ILE:HG12	2.35	0.52
1:E:2213:LYS:O	1:E:2215:LEU:HD23	2.08	0.52
1:G:2023:TYR:O	1:G:2027:THR:HG23	2.10	0.52
2:H:128:GLU:HB3	2:H:145:MSE:HE2	1.91	0.52
1:A:2362:ILE:HG22	1:A:2370:TRP:CG	2.44	0.52
2:D:17:PHE:C	2:D:17:PHE:CD2	2.88	0.52
2:D:118:THR:O	2:D:122:VAL:HG23	2.10	0.52
1:E:2138:GLN:O	1:E:2141:LEU:HB3	2.10	0.52
2:F:48:GLU:OE1	2:F:76:LYS:NZ	2.40	0.52
2:F:13:PHE:CD1	2:F:13:PHE:N	2.75	0.51
1:G:2006:VAL:HB	1:G:2140:GLN:HE22	1.75	0.51
1:C:2093:ILE:HD11	1:C:2213:LYS:HG2	1.91	0.51
1:A:2329:PHE:CD1	1:A:2329:PHE:C	2.89	0.51
1:C:2334:PHE:CD2	1:C:2340:MSE:HG2	2.45	0.51
2:B:52:MSE:HB3	2:B:72:MSE:SE	2.61	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:LEU:HD23	2:D:126:ILE:CD1	2.40	0.51
1:G:2150:PHE:O	1:G:2153:THR:HG23	2.11	0.51
1:G:2187:LEU:HB3	1:G:2188:PRO:HD3	1.91	0.51
1:A:2132:ASP:OD1	1:A:2133:PRO:CD	2.58	0.51
1:C:2137:GLU:OE2	1:C:2140:GLN:OE1	2.29	0.51
1:E:2358:ARG:H	1:E:2358:ARG:CD	2.20	0.51
1:A:2098:GLN:HE22	1:A:2217:ALA:HB1	1.75	0.51
1:C:2349:ASN:HB3	1:C:2364:GLN:HB3	1.93	0.51
2:D:107:ARG:NH2	2:D:123:ASP:OD1	2.44	0.51
1:E:1992:THR:OG1	1:E:1995:TYR:HB3	2.10	0.51
1:E:2166:ASN:O	1:E:2199:VAL:HG13	2.10	0.51
1:G:2190:LEU:HB3	1:G:2202:ILE:HD11	1.93	0.51
1:C:1968:SER:HB3	1:C:1971:ALA:HB2	1.93	0.51
1:E:2240:HIS:HA	1:E:2243:GLN:CG	2.40	0.51
1:E:2326:ILE:O	1:E:2330:ILE:HG13	2.11	0.51
2:F:44:PRO:HB3	2:F:76:LYS:HD3	1.91	0.51
1:A:2138:GLN:NE2	1:A:2138:GLN:CA	2.74	0.51
2:B:100:TYR:HE2	2:B:138:ASN:HB2	1.72	0.51
1:E:2126:TRP:CG	1:E:2130:PHE:HE1	2.29	0.51
1:A:2207:LYS:N	1:A:2212:TYR:OH	2.35	0.50
2:B:128:GLU:CB	2:B:145:MSE:HE1	2.42	0.50
2:B:84:GLU:HG2	2:B:87:ARG:HH12	1.75	0.50
1:A:2177:ARG:HH11	1:A:2177:ARG:CG	2.24	0.50
1:A:2233:VAL:HG12	1:A:2234:ARG:N	2.26	0.50
1:C:2273:LEU:CD2	2:D:125:MSE:HE1	2.42	0.50
2:D:103:ALA:HA	2:D:137:VAL:HG23	1.92	0.50
2:F:120:GLU:HA	2:F:123:ASP:HB2	1.93	0.50
1:G:2177:ARG:HH11	1:G:2180:ASN:HB3	1.76	0.50
1:A:2158:SER:OG	1:A:2185:VAL:HB	2.12	0.50
2:D:30:THR:CG2	2:D:64:ILE:CG1	2.75	0.50
1:A:2345:PHE:O	1:A:2351:VAL:HA	2.10	0.50
1:C:2343:GLU:OE1	1:C:2354:HIS:NE2	2.44	0.50
1:G:2119:LEU:HD23	1:G:2119:LEU:N	2.26	0.50
2:H:37:MSE:HE1	2:H:44:PRO:HG3	1.92	0.50
1:A:2020:MSE:HE2	1:A:2119:LEU:HB3	1.84	0.50
1:E:2364:GLN:HA	1:E:2367:ASP:O	2.11	0.50
2:H:17:PHE:HD1	2:H:69:PHE:CE1	2.30	0.50
1:E:2094:LEU:HB3	1:E:2104:VAL:HG11	1.94	0.50
1:G:1970:VAL:HG13	1:G:2063:GLU:OE1	2.10	0.50
1:C:1968:SER:HB3	1:C:1971:ALA:CB	2.42	0.50
1:G:1970:VAL:CG1	1:G:2069:PHE:CD1	2.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2087:PHE:HB2	1:A:2106:TYR:CE1	2.47	0.49
1:E:2004:VAL:HG11	1:E:2144:SER:CA	2.39	0.49
1:E:2039:LEU:HD13	1:E:2065:TYR:CE2	2.47	0.49
1:A:2329:PHE:CD2	1:A:2362:ILE:HD11	2.47	0.49
1:A:2349:ASN:HD22	1:A:2364:GLN:NE2	2.10	0.49
1:C:2012:VAL:O	1:C:2016:MSE:HG3	2.11	0.49
2:B:44:PRO:HG2	2:B:49:LEU:HD13	1.90	0.49
1:A:2136:ALA:HB3	1:E:2136:ALA:HB2	1.94	0.49
2:B:139:TYR:HD1	2:B:139:TYR:H	1.60	0.49
1:C:2352:LEU:HD12	1:C:2352:LEU:C	2.36	0.49
1:E:2051:ASP:HB3	1:E:2054:LYS:CB	2.37	0.49
1:E:2367:ASP:O	1:E:2367:ASP:OD1	2.30	0.49
1:G:2328:ARG:NH2	2:H:40:LEU:CD2	2.64	0.49
1:C:2171:ILE:N	1:C:2171:ILE:HD12	2.27	0.49
1:C:2264:VAL:CG1	2:D:92:VAL:HG21	2.27	0.49
1:E:2013:LYS:C	1:E:2017:ILE:HG13	2.36	0.49
1:E:2057:GLU:O	1:E:2061:LYS:HB2	2.12	0.49
1:A:2021:SER:HA	1:A:2024:ILE:HD12	1.95	0.49
2:B:131:ILE:HG13	2:B:132:ASP:N	2.27	0.49
2:B:147:THR:O	2:B:147:THR:HG22	2.13	0.49
1:C:2272:MSE:HE1	2:D:90:PHE:HE2	1.78	0.49
1:A:2290:VAL:HG22	1:A:2299:VAL:HG22	1.94	0.49
2:B:17:PHE:CE2	2:B:28:ILE:HD13	2.48	0.49
1:E:2233:VAL:O	1:E:2259:LEU:HA	2.12	0.49
2:F:94:ASP:OD2	2:F:98:ASN:O	2.30	0.49
1:G:2129:LEU:CD1	1:G:2130:PHE:CZ	2.91	0.49
2:H:137:VAL:O	2:H:137:VAL:HG12	2.12	0.49
2:F:44:PRO:HG2	2:F:49:LEU:CD1	2.38	0.49
1:G:2349:ASN:CB	1:G:2364:GLN:OE1	2.61	0.49
2:H:13:PHE:CD1	2:H:13:PHE:N	2.80	0.49
1:A:2288:LEU:HD23	1:A:2337:PHE:HB2	1.95	0.49
1:C:2006:VAL:CG2	1:C:2140:GLN:HG2	2.38	0.49
1:C:2205:LEU:HD11	1:C:2220:ILE:HG22	1.94	0.49
2:D:121:GLU:O	2:D:125:MSE:HG3	2.12	0.49
2:D:132:ASP:HB2	2:D:134:ASP:OD1	2.12	0.49
2:F:91:ARG:HG3	2:F:139:TYR:OH	2.12	0.49
1:G:1997:PRO:HA	4:G:2401:HOH:O	2.13	0.49
2:H:13:PHE:O	2:H:17:PHE:HB2	2.12	0.49
2:D:83:GLU:OE1	2:D:87:ARG:NH1	2.45	0.48
2:H:20:PHE:O	2:H:28:ILE:HG12	2.13	0.48
1:A:2136:ALA:HB3	1:E:2136:ALA:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2052:TRP:O	1:C:2056:VAL:HG23	2.13	0.48
1:E:2008:VAL:CG1	1:E:2009:SER:N	2.76	0.48
1:G:2224:LEU:N	1:G:2224:LEU:HD12	2.28	0.48
2:H:128:GLU:HB3	2:H:145:MSE:CE	2.43	0.48
1:A:2362:ILE:HG22	1:A:2370:TRP:CA	2.43	0.48
1:C:2195:ARG:NH2	2:D:111:THR:HG23	2.27	0.48
1:E:1996:VAL:CG2	1:E:2052:TRP:CZ3	2.96	0.48
1:G:2233:VAL:CG1	1:G:2234:ARG:N	2.75	0.48
1:G:2337:PHE:CD1	1:G:2337:PHE:C	2.90	0.48
2:H:38:ARG:HA	2:H:42:GLN:O	2.12	0.48
1:A:2037:GLU:OE1	1:A:2037:GLU:HA	2.13	0.48
1:A:2212:TYR:HA	1:A:2215:LEU:HD22	1.95	0.48
1:A:2281:SER:HB2	1:A:2327:GLU:OE2	2.13	0.48
1:C:2006:VAL:HG11	1:C:2140:GLN:O	2.12	0.48
2:D:102:SER:HB2	2:D:105:GLU:CG	2.43	0.48
2:D:129:ALA:HB2	2:D:142:PHE:CE1	2.48	0.48
1:E:1985:ASP:OD2	1:E:1990:VAL:N	2.46	0.48
1:E:2358:ARG:N	1:E:2358:ARG:HH21	2.00	0.48
1:A:2131:LEU:HD11	1:A:2138:GLN:CB	2.33	0.48
1:A:2136:ALA:O	1:A:2140:GLN:HG2	2.13	0.48
2:D:65:ASP:HB2	2:D:67:PRO:HG2	1.96	0.48
2:F:107:ARG:NH2	2:F:123:ASP:OD1	2.46	0.48
1:G:2266:LEU:HD23	1:G:2266:LEU:C	2.38	0.48
1:A:1987:ASP:OD2	2:B:103:ALA:HB1	2.14	0.48
1:A:2014:GLN:NE2	1:A:2018:GLN:NE2	2.61	0.48
1:A:2090:TYR:CZ	1:A:2209:VAL:HG22	2.49	0.48
1:C:2233:VAL:CG1	1:C:2234:ARG:N	2.77	0.48
2:H:91:ARG:HG3	2:H:139:TYR:OH	2.13	0.48
2:D:100:TYR:CE2	2:D:138:ASN:HA	2.49	0.48
2:H:129:ALA:HB2	2:H:142:PHE:CD1	2.48	0.48
1:A:1994:LYS:O	1:A:2052:TRP:HB2	2.13	0.48
1:A:2322:GLN:OE1	1:A:2346:LEU:HG	2.14	0.48
2:F:147:THR:HG22	2:F:147:THR:O	2.13	0.48
1:E:2187:LEU:N	1:E:2188:PRO:CD	2.77	0.48
1:G:2177:ARG:HB3	1:G:2180:ASN:ND2	2.27	0.48
1:E:2362:ILE:O	1:E:2362:ILE:HG13	2.14	0.47
1:G:2227:ALA:HB1	2:H:45:THR:HG22	1.95	0.47
1:G:2351:VAL:HB	1:G:2362:ILE:HG12	1.95	0.47
1:A:2026:HIS:O	1:E:2250:ASN:O	2.32	0.47
1:G:2051:ASP:HB3	1:G:2054:LYS:HB2	1.94	0.47
1:G:2091:ARG:HG2	1:G:2104:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1994:LYS:O	1:A:2052:TRP:CB	2.62	0.47
1:A:2032:PRO:HB3	1:A:2033:LYS:HE2	1.95	0.47
2:B:87:ARG:HD3	2:B:140:GLU:HG2	1.94	0.47
2:F:44:PRO:CB	2:F:49:LEU:HD11	2.44	0.47
1:G:2098:GLN:NE2	1:G:2217:ALA:HB1	2.28	0.47
2:D:101:ILE:HG12	2:D:139:TYR:CD1	2.46	0.47
1:E:2020:MSE:CE	1:E:2119:LEU:O	2.56	0.47
2:F:17:PHE:CZ	2:F:28:ILE:HG23	2.49	0.47
1:A:2365:LYS:O	1:A:2366:GLU:OE1	2.32	0.47
1:G:2233:VAL:CG1	1:G:2234:ARG:H	2.28	0.47
2:H:30:THR:OG1	2:H:33:LEU:CD2	2.62	0.47
1:A:2213:LYS:O	1:A:2215:LEU:CD1	2.62	0.47
1:C:2282:LEU:N	1:C:2282:LEU:HD23	2.29	0.47
2:D:103:ALA:HA	2:D:137:VAL:CG2	2.45	0.47
1:E:2098:GLN:HE22	1:E:2217:ALA:HB1	1.78	0.47
1:C:1992:THR:HG22	1:C:1995:TYR:HB3	1.96	0.47
2:D:25:ASP:HA	2:H:61:ASN:CB	2.43	0.47
1:E:2326:ILE:CD1	1:E:2346:LEU:CB	2.66	0.47
2:F:118:THR:O	2:F:122:VAL:HG23	2.14	0.47
1:G:1983:TRP:O	1:G:1986:THR:HG23	2.13	0.47
1:G:1998:VAL:HG12	1:G:2001:PHE:CD1	2.50	0.47
2:H:30:THR:CB	2:H:33:LEU:HD23	2.44	0.47
1:C:2233:VAL:CG1	1:C:2234:ARG:H	2.27	0.47
1:E:2179:GLY:HA2	1:E:2184:ASN:HD21	1.80	0.47
2:H:66:PHE:HZ	2:H:70:LEU:HD13	1.79	0.47
1:C:2365:LYS:O	1:C:2366:GLU:HB2	2.14	0.47
1:A:2032:PRO:HB2	1:A:2035:GLN:CB	2.40	0.47
1:A:2136:ALA:HB3	1:E:2136:ALA:CB	2.44	0.47
2:F:117:LEU:HD12	2:F:117:LEU:HA	1.72	0.47
2:H:17:PHE:C	2:H:17:PHE:CD2	2.92	0.47
2:H:99:GLY:HA2	2:H:139:TYR:CE1	2.50	0.47
1:C:2139:ASN:O	1:C:2143:SER:N	2.37	0.46
1:E:2195:ARG:HH12	2:F:111:THR:HG23	1.81	0.46
1:E:2242:ARG:HD3	1:E:2242:ARG:HA	1.66	0.46
1:G:1982:ARG:O	1:G:1986:THR:HG23	2.15	0.46
2:B:132:ASP:CB	2:B:134:ASP:OD1	2.63	0.46
1:E:2069:PHE:HA	1:E:2110:VAL:CG1	2.45	0.46
1:A:2329:PHE:CA	2:B:19:LEU:HD23	2.44	0.46
2:B:6:THR:HG1	2:B:9:GLN:HG3	1.80	0.46
1:C:1998:VAL:HB	1:C:2001:PHE:HB2	1.97	0.46
1:G:2233:VAL:CG2	1:G:2262:LEU:HD11	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2132:ASP:OD1	1:A:2134:ASP:HB2	2.15	0.46
1:A:2175:GLY:H	1:A:2206:ASP:HB2	1.81	0.46
1:C:2190:LEU:HB3	1:C:2202:ILE:HD11	1.95	0.46
1:E:2051:ASP:CB	1:E:2054:LYS:HG3	2.45	0.46
1:G:1973:ARG:CG	1:G:1973:ARG:HH21	2.29	0.46
2:H:30:THR:OG1	2:H:33:LEU:HD23	2.15	0.46
2:D:94:ASP:HA	2:D:101:ILE:HG22	1.97	0.46
1:E:2149:THR:O	1:E:2152:ASN:HB2	2.16	0.46
1:G:2150:PHE:HA	1:G:2153:THR:CG2	2.46	0.46
1:G:2233:VAL:HG12	1:G:2234:ARG:H	1.81	0.46
1:C:2302:TRP:CG	1:C:2303:PRO:HA	2.51	0.46
1:A:2046:SER:OG	1:A:2055:ARG:HG3	2.15	0.46
1:A:2218:ASP:OD2	1:A:2218:ASP:N	2.39	0.46
2:B:62:GLY:O	2:B:63:THR:OG1	2.31	0.46
1:C:2020:MSE:HE1	1:C:2123:LEU:HB2	1.98	0.46
1:E:2171:ILE:N	1:E:2171:ILE:HD12	2.30	0.46
1:A:2314:LEU:CD2	1:A:2346:LEU:HB3	2.46	0.46
1:C:2130:PHE:O	1:C:2138:GLN:OE1	2.34	0.46
2:F:57:ASP:OD1	2:F:57:ASP:O	2.33	0.46
1:G:2073:HIS:ND1	1:G:2073:HIS:N	2.61	0.46
2:F:6:THR:HB	2:F:9:GLN:HG3	1.98	0.46
1:E:2044:VAL:O	1:E:2048:LEU:HG	2.15	0.46
1:E:2130:PHE:CD1	1:E:2130:PHE:N	2.81	0.46
1:G:2349:ASN:CA	1:G:2364:GLN:OE1	2.64	0.46
1:G:2370:TRP:HZ2	2:H:19:LEU:HA	1.81	0.46
2:H:69:PHE:HE2	2:H:73:MSE:CE	2.28	0.46
1:C:2229:VAL:O	1:C:2229:VAL:HG13	2.17	0.45
2:F:13:PHE:O	2:F:17:PHE:HB2	2.15	0.45
2:F:30:THR:CB	2:F:62:GLY:HA2	2.46	0.45
2:H:37:MSE:HG2	2:H:73:MSE:HE2	1.97	0.45
1:A:2352:LEU:HD23	1:A:2360:ARG:CA	2.43	0.45
1:C:2349:ASN:O	1:C:2364:GLN:HB2	2.16	0.45
2:D:66:PHE:N	2:D:67:PRO:CD	2.77	0.45
2:D:71:THR:O	2:D:74:ALA:N	2.49	0.45
1:E:2067:TYR:HB3	1:E:2112:GLY:HA2	1.99	0.45
1:E:2141:LEU:C	1:E:2141:LEU:CD1	2.88	0.45
1:E:2223:ARG:NH2	1:E:2284:THR:O	2.42	0.45
1:A:2206:ASP:OD2	1:A:2222:ARG:NH1	2.46	0.45
1:A:2294:GLU:O	1:A:2295:GLU:CG	2.63	0.45
1:A:2302:TRP:CG	1:A:2303:PRO:HA	2.51	0.45
2:D:87:ARG:O	2:D:91:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:TYR:CD2	2:D:138:ASN:HA	2.52	0.45
2:H:121:GLU:O	2:H:124:GLN:HG2	2.17	0.45
1:A:2289:LEU:HD23	1:A:2304:GLY:HA3	1.97	0.45
1:A:2353:SER:O	1:A:2354:HIS:HD2	2.00	0.45
1:C:2286:ARG:HB3	1:C:2288:LEU:CD1	2.46	0.45
1:G:1973:ARG:NH2	1:G:2159:VAL:O	2.49	0.45
1:G:2072:PRO:HG2	1:G:2073:HIS:ND1	2.31	0.45
2:H:107:ARG:NH2	2:H:123:ASP:OD1	2.49	0.45
1:E:2210:SER:HA	1:E:2213:LYS:HG3	1.97	0.45
2:F:48:GLU:CD	2:F:76:LYS:NZ	2.75	0.45
2:F:94:ASP:OD2	2:F:139:TYR:HE1	2.00	0.45
1:G:2025:GLU:O	1:G:2033:LYS:HE3	2.16	0.45
1:C:2177:ARG:HB3	1:C:2180:ASN:HD22	1.81	0.45
1:A:2358:ARG:HE	1:A:2358:ARG:C	2.25	0.45
1:C:1992:THR:HG23	1:C:1995:TYR:H	1.82	0.45
1:E:2073:HIS:CD2	1:E:2103:LYS:HB2	2.52	0.45
2:H:19:LEU:N	2:H:19:LEU:HD23	2.31	0.45
2:H:107:ARG:HH22	2:H:123:ASP:HA	1.82	0.45
1:A:1969:LEU:HD23	1:A:1969:LEU:N	2.31	0.45
1:A:2008:VAL:HG11	1:A:2013:LYS:HE3	1.99	0.45
1:A:2362:ILE:HG21	1:A:2370:TRP:CE2	2.52	0.45
1:E:2132:ASP:OD1	1:E:2132:ASP:C	2.60	0.45
1:E:2231:VAL:HG11	1:E:2266:LEU:HD13	1.98	0.45
2:F:145:MSE:O	2:F:145:MSE:HG2	2.17	0.45
1:G:2005:ASP:OD1	1:G:2050:TYR:CD2	2.70	0.45
2:H:124:GLN:O	2:H:128:GLU:CG	2.60	0.45
1:A:2323:GLN:O	1:A:2327:GLU:HB2	2.17	0.45
1:C:2351:VAL:HB	1:C:2362:ILE:HG13	1.99	0.45
1:E:2330:ILE:HD13	1:E:2340:MSE:HE3	1.99	0.45
1:A:2052:TRP:O	1:A:2056:VAL:HG23	2.17	0.45
1:A:2132:ASP:CG	1:A:2134:ASP:HB2	2.42	0.45
1:C:2206:ASP:OD1	1:C:2222:ARG:NH1	2.50	0.45
1:C:2310:LYS:NZ	1:C:2340:MSE:O	2.47	0.45
1:C:2315:ASP:OD2	1:C:2315:ASP:C	2.60	0.45
2:D:46:GLU:HA	2:D:49:LEU:HD12	1.99	0.45
1:G:2207:LYS:HB3	1:G:2208:PRO:CD	2.42	0.45
1:A:1991:ALA:HB2	1:A:1997:PRO:CD	2.47	0.44
1:A:2001:PHE:CE2	1:A:2150:PHE:O	2.70	0.44
1:E:2336:ASN:OD1	1:E:2339:GLN:NE2	2.50	0.44
1:G:2288:LEU:CD2	1:G:2337:PHE:HB2	2.47	0.44
1:E:2309:SER:HB3	1:G:2099:THR:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:GLU:O	2:F:88:GLU:HG2	2.17	0.44
1:A:2245:GLU:O	1:A:2249:ASP:N	2.49	0.44
1:E:2008:VAL:HG12	1:E:2009:SER:H	1.81	0.44
1:E:2158:SER:OG	1:E:2185:VAL:HB	2.17	0.44
2:F:13:PHE:N	2:F:13:PHE:HD1	2.14	0.44
1:G:2132:ASP:OD1	1:G:2132:ASP:N	2.50	0.44
2:H:98:ASN:ND2	2:H:99:GLY:O	2.50	0.44
1:C:2345:PHE:CD1	1:C:2352:LEU:HD11	2.53	0.44
1:E:2218:ASP:OD1	1:E:2218:ASP:N	2.38	0.44
1:G:2279:PHE:CZ	1:G:2323:GLN:HG2	2.53	0.44
1:G:2299:VAL:CG2	1:G:2312:ILE:CD1	2.95	0.44
1:E:1990:VAL:HG12	1:E:1997:PRO:HG3	1.99	0.44
1:G:2178:LEU:HD12	1:G:2233:VAL:CG2	2.48	0.44
1:G:2314:LEU:HD11	1:G:2326:ILE:HG21	1.98	0.44
2:H:69:PHE:O	2:H:69:PHE:CD2	2.68	0.44
2:H:98:ASN:C	2:H:98:ASN:HD22	2.25	0.44
1:A:2187:LEU:HB3	1:A:2188:PRO:HD3	2.00	0.44
1:C:2016:MSE:HE1	1:C:2141:LEU:HD11	2.00	0.44
1:C:2016:MSE:HE2	1:C:2141:LEU:HD11	2.00	0.44
1:E:2087:PHE:CD2	1:E:2087:PHE:N	2.76	0.44
1:G:2046:SER:CB	1:G:2054:LYS:HB3	2.48	0.44
1:G:2351:VAL:HB	1:G:2362:ILE:CG1	2.48	0.44
1:A:2368:GLY:N	2:B:18:SER:HB3	2.33	0.44
1:E:2008:VAL:CG1	1:E:2009:SER:H	2.31	0.44
1:E:2224:LEU:N	1:E:2224:LEU:CD1	2.80	0.44
1:G:2184:ASN:HD22	1:G:2184:ASN:HA	1.64	0.44
1:E:2039:LEU:HD13	1:E:2065:TYR:HE2	1.82	0.44
1:G:2349:ASN:HB3	1:G:2364:GLN:OE1	2.17	0.44
2:B:54:ASN:O	2:B:57:ASP:OD1	2.36	0.44
2:D:139:TYR:O	2:D:139:TYR:CD2	2.69	0.44
1:A:2135:ASN:C	1:A:2135:ASN:OD1	2.61	0.43
1:A:2310:LYS:NZ	1:A:2340:MSE:O	2.49	0.43
1:E:2362:ILE:HG21	1:E:2370:TRP:CZ3	2.52	0.43
1:G:1973:ARG:CG	1:G:1973:ARG:NH2	2.81	0.43
2:H:66:PHE:HB3	2:H:67:PRO:HD3	1.99	0.43
1:C:2212:TYR:HA	1:C:2215:LEU:HD12	1.98	0.43
1:C:2234:ARG:HH21	1:C:2257:ASP:HB2	1.81	0.43
2:D:13:PHE:N	2:D:13:PHE:CD1	2.84	0.43
1:E:2234:ARG:HD2	1:E:2257:ASP:HA	2.00	0.43
1:G:2224:LEU:HD12	1:G:2224:LEU:H	1.82	0.43
1:A:2014:GLN:HA	1:A:2017:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2217:ALA:HA	1:A:2220:ILE:CD1	2.47	0.43
2:B:19:LEU:O	2:B:20:PHE:HB2	2.17	0.43
2:B:134:ASP:OD1	2:B:134:ASP:N	2.43	0.43
2:D:103:ALA:HB2	2:D:135:GLY:O	2.19	0.43
2:D:131:ILE:HG12	2:D:141:GLU:CD	2.42	0.43
1:E:2040:ALA:O	1:E:2044:VAL:HG22	2.18	0.43
1:G:2016:MSE:HE1	1:G:2145:ILE:HD11	1.91	0.43
1:G:2280:TYR:CD2	1:G:2280:TYR:C	2.96	0.43
1:G:2315:ASP:C	1:G:2315:ASP:OD2	2.61	0.43
1:E:2158:SER:O	1:E:2162:THR:HG23	2.18	0.43
1:C:2345:PHE:HB2	1:C:2352:LEU:CD1	2.48	0.43
2:D:6:THR:O	2:D:10:ILE:HG13	2.17	0.43
1:E:2020:MSE:HB3	1:E:2040:ALA:HB1	2.01	0.43
1:E:2345:PHE:O	1:E:2351:VAL:HA	2.18	0.43
1:G:2001:PHE:CD1	1:G:2001:PHE:N	2.87	0.43
1:G:2351:VAL:H	1:G:2362:ILE:HB	1.82	0.43
1:C:2120:ASN:O	1:C:2124:MSE:HG3	2.19	0.43
1:C:2149:THR:O	1:C:2152:ASN:HB2	2.19	0.43
1:E:2315:ASP:OD2	1:E:2315:ASP:C	2.62	0.43
1:G:2023:TYR:O	1:G:2027:THR:CG2	2.67	0.43
1:A:2014:GLN:HE22	1:A:2018:GLN:HG3	1.75	0.43
1:C:2370:TRP:HE1	2:D:22:LYS:HG2	1.82	0.43
2:D:45:THR:HG22	2:D:48:GLU:HB2	2.01	0.43
2:B:138:ASN:HB3	2:B:141:GLU:CB	2.38	0.43
1:E:2022:GLY:O	1:E:2025:GLU:HB3	2.19	0.43
1:E:2250:ASN:OD1	1:E:2250:ASN:C	2.62	0.43
1:A:1973:ARG:O	1:A:1977:VAL:HG23	2.19	0.43
1:A:1994:LYS:HD3	1:A:2051:ASP:OD2	2.18	0.43
1:C:2128:GLY:CA	1:C:2131:LEU:HB3	2.37	0.43
1:C:2315:ASP:HB3	1:C:2322:GLN:HE22	1.83	0.43
1:A:2094:LEU:CD2	1:A:2220:ILE:HG21	2.49	0.43
1:C:1985:ASP:O	1:C:1985:ASP:CG	2.62	0.43
1:C:2187:LEU:N	1:C:2188:PRO:CD	2.82	0.43
1:A:2167:ASP:OD2	1:A:2203:ARG:NH1	2.52	0.42
1:A:2213:LYS:O	1:A:2215:LEU:HD12	2.19	0.42
1:C:2194:GLN:HG2	1:C:2199:VAL:HG12	2.01	0.42
1:E:2354:HIS:HE1	1:E:2356:ASP:O	2.01	0.42
1:G:2047:THR:O	1:G:2148:ALA:HB1	2.19	0.42
1:A:1982:ARG:NH1	1:A:1992:THR:O	2.52	0.42
1:A:2094:LEU:HD21	1:A:2220:ILE:HG21	2.01	0.42
1:A:2182:PHE:HA	1:A:2186:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2266:LEU:HG	2:F:113:LEU:HD11	2.00	0.42
1:G:2063:GLU:HA	1:G:2067:TYR:O	2.19	0.42
2:H:44:PRO:CB	2:H:76:LYS:HE2	2.47	0.42
1:A:2012:VAL:HG12	1:A:2016:MSE:HE2	2.01	0.42
1:A:2177:ARG:CG	1:A:2177:ARG:NH1	2.82	0.42
1:A:2247:LEU:HD12	1:A:2247:LEU:HA	1.83	0.42
1:C:1970:VAL:HG23	1:C:2063:GLU:OE1	2.18	0.42
1:C:1987:ASP:OD2	2:D:107:ARG:NH1	2.51	0.42
2:D:129:ALA:HA	2:D:145:MSE:HE1	2.02	0.42
1:E:2058:PHE:O	1:E:2062:LEU:HG	2.19	0.42
1:G:2131:LEU:HD13	1:G:2131:LEU:H	1.78	0.42
2:H:44:PRO:CG	2:H:49:LEU:HD12	2.50	0.42
1:A:2273:LEU:HD23	1:A:2277:LEU:HD13	2.01	0.42
1:C:2233:VAL:CG2	1:C:2262:LEU:CD1	2.96	0.42
2:D:141:GLU:C	2:D:145:MSE:HE3	2.44	0.42
1:G:2315:ASP:N	1:G:2322:GLN:NE2	2.68	0.42
1:G:2332:ALA:HB1	2:H:19:LEU:O	2.19	0.42
1:A:2298:GLU:HB2	1:A:2300:ARG:HH12	1.85	0.42
2:B:66:PHE:N	2:B:67:PRO:CD	2.80	0.42
1:C:2277:LEU:HA	1:C:2278:PRO:HD3	1.92	0.42
1:E:2314:LEU:HD23	1:E:2346:LEU:HB3	2.01	0.42
1:G:2129:LEU:HD12	1:G:2130:PHE:CE2	2.53	0.42
1:A:2349:ASN:HB3	1:A:2364:GLN:HB3	2.02	0.42
1:A:2051:ASP:CB	1:A:2054:LYS:HD2	2.50	0.42
1:C:2264:VAL:CG2	1:C:2266:LEU:HD11	2.48	0.42
1:C:1968:SER:OG	1:C:2063:GLU:OE2	2.38	0.42
2:F:110:MSE:HE2	2:F:125:MSE:HE1	2.01	0.42
2:H:17:PHE:CE1	2:H:66:PHE:HA	2.55	0.42
1:C:2194:GLN:NE2	1:C:2200:GLY:O	2.53	0.42
1:E:2281:SER:O	1:E:2285:GLU:CG	2.68	0.42
1:C:2138:GLN:O	1:C:2141:LEU:HB3	2.20	0.42
2:D:70:LEU:HD13	2:D:70:LEU:O	2.20	0.42
1:E:2082:TRP:O	1:E:2082:TRP:CG	2.72	0.42
2:F:125:MSE:HE3	2:F:142:PHE:HZ	1.85	0.42
1:G:2001:PHE:HD2	1:G:2150:PHE:HD1	1.67	0.42
2:H:28:ILE:CG2	2:H:29:THR:N	2.83	0.42
1:A:2073:HIS:HB2	1:A:2077:SER:HB3	2.02	0.41
1:C:2345:PHE:HB2	1:C:2352:LEU:HG	2.01	0.41
1:E:2135:ASN:ND2	1:E:2135:ASN:C	2.78	0.41
1:A:2033:LYS:HD3	1:A:2033:LYS:N	2.13	0.41
1:E:2020:MSE:HE3	1:E:2123:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2008:VAL:HG12	1:G:2012:VAL:HB	2.02	0.41
1:G:2324:LYS:O	1:G:2328:ARG:HG3	2.20	0.41
2:D:83:GLU:OE1	2:D:87:ARG:NE	2.52	0.41
2:D:145:MSE:O	2:D:145:MSE:HG2	2.17	0.41
1:E:2240:HIS:O	1:E:2241:GLU:C	2.62	0.41
2:F:94:ASP:OD2	2:F:139:TYR:CE1	2.73	0.41
1:A:2184:ASN:HD22	1:A:2184:ASN:HA	1.64	0.41
1:A:2315:ASP:OD2	1:A:2315:ASP:C	2.63	0.41
1:C:2351:VAL:CG2	1:C:2362:ILE:HD12	2.49	0.41
2:D:134:ASP:OD1	2:D:134:ASP:N	2.53	0.41
1:E:2187:LEU:HB3	1:E:2188:PRO:HD3	2.02	0.41
2:F:30:THR:HB	2:F:62:GLY:CA	2.49	0.41
1:G:2302:TRP:CD2	1:G:2303:PRO:HA	2.56	0.41
1:A:2361:ILE:C	1:A:2362:ILE:HG23	2.46	0.41
1:C:2215:LEU:HD22	1:C:2219:GLN:CD	2.45	0.41
1:E:1970:VAL:CG1	1:E:2069:PHE:CD1	2.99	0.41
1:E:2051:ASP:HB3	1:E:2054:LYS:HG3	2.01	0.41
1:E:2076:LYS:HD3	1:E:2102:LYS:HE3	2.03	0.41
1:E:2193:LEU:HD13	1:E:2199:VAL:CG2	2.50	0.41
2:F:123:ASP:O	2:F:127:ARG:HG3	2.20	0.41
1:G:2137:GLU:HG2	1:G:2138:GLN:CD	2.46	0.41
1:A:2193:LEU:HD23	1:A:2193:LEU:HA	1.90	0.41
1:E:2233:VAL:CG1	1:E:2234:ARG:N	2.71	0.41
1:G:2117:ILE:CG2	1:G:2121:LYS:HE3	2.51	0.41
2:B:90:PHE:HB3	2:B:139:TYR:CD2	2.46	0.41
2:D:6:THR:HB	2:D:9:GLN:HB2	2.03	0.41
2:D:129:ALA:HB2	2:D:142:PHE:HD1	1.83	0.41
1:E:2251:PRO:O	1:E:2252:ASP:OD1	2.38	0.41
2:H:114:GLY:HA3	2:H:117:LEU:HD12	2.03	0.41
1:A:2001:PHE:CD2	1:A:2151:SER:HA	2.56	0.41
2:B:81:ASP:O	2:B:85:GLU:HG3	2.21	0.41
2:D:14:LYS:HA	2:D:66:PHE:CZ	2.55	0.41
1:E:2281:SER:OG	1:E:2327:GLU:OE2	2.39	0.41
1:E:2310:LYS:HD2	1:E:2337:PHE:CE2	2.56	0.41
1:A:1970:VAL:CG1	1:A:2069:PHE:HB2	2.50	0.41
2:D:109:VAL:HG12	2:D:110:MSE:HE2	2.03	0.41
1:E:2271:SER:HA	1:E:2274:ARG:HD3	2.03	0.41
1:E:2300:ARG:HH12	1:G:2096:ASN:ND2	2.19	0.41
1:G:2005:ASP:OD1	1:G:2050:TYR:HE2	2.04	0.41
1:G:2231:VAL:HG12	1:G:2262:LEU:HD12	2.02	0.41
1:A:1977:VAL:HG13	1:A:1981:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2227:ALA:HB1	2:F:45:THR:HG22	2.03	0.41
2:F:52:MSE:HG2	2:F:72:MSE:SE	2.71	0.41
1:G:1970:VAL:HG12	1:G:2069:PHE:HB2	2.03	0.41
2:H:83:GLU:HB3	2:H:87:ARG:NH1	2.36	0.41
1:A:2314:LEU:HD23	1:A:2346:LEU:HB3	2.03	0.40
1:C:2273:LEU:HD13	2:D:117:LEU:CD1	2.51	0.40
1:C:2281:SER:O	1:C:2285:GLU:HG2	2.21	0.40
2:D:37:MSE:HG2	2:D:73:MSE:HE3	2.03	0.40
1:E:2058:PHE:CZ	1:E:2062:LEU:HD11	2.57	0.40
1:A:2174:GLY:O	1:A:2232:LYS:HE3	2.21	0.40
2:B:18:SER:O	2:B:21:ASP:HB2	2.22	0.40
1:C:1978:ALA:HB2	1:C:2052:TRP:CZ2	2.56	0.40
1:G:2141:LEU:HD12	1:G:2144:SER:OG	2.21	0.40
1:G:2314:LEU:HD23	1:G:2322:GLN:HG2	2.04	0.40
2:H:5:LEU:HD21	2:H:71:THR:OG1	2.21	0.40
1:A:2055:ARG:NH1	1:A:2152:ASN:HD22	2.19	0.40
1:A:2152:ASN:HB3	1:A:2156:TRP:CH2	2.57	0.40
1:C:2189:ALA:O	1:C:2192:GLN:HB3	2.22	0.40
2:D:10:ILE:CD1	2:D:70:LEU:HD11	2.51	0.40
2:D:103:ALA:CA	2:D:137:VAL:HG23	2.51	0.40
1:E:2094:LEU:HD21	1:E:2220:ILE:HG21	2.04	0.40
2:F:61:ASN:O	2:F:61:ASN:ND2	2.55	0.40
2:H:30:THR:HB	2:H:64:ILE:HG12	2.01	0.40
1:A:2009:SER:O	1:A:2009:SER:OG	2.39	0.40
1:A:2298:GLU:HB3	1:A:2300:ARG:CZ	2.51	0.40
1:A:2310:LYS:HD2	1:A:2337:PHE:CE2	2.56	0.40
1:A:2361:ILE:O	1:A:2362:ILE:HG23	2.21	0.40
1:C:1970:VAL:HG22	1:C:2069:PHE:HB2	2.04	0.40
1:C:2016:MSE:HG2	1:C:2126:TRP:CZ3	2.56	0.40
2:D:29:THR:CG2	2:D:32:GLU:OE1	2.70	0.40
1:E:2311:THR:OG1	1:E:2343:GLU:HG3	2.22	0.40
1:G:2041:THR:O	1:G:2045:GLU:HG3	2.22	0.40
1:A:1998:VAL:HB	1:A:2001:PHE:HB2	2.02	0.40
1:A:2193:LEU:HB3	1:A:2199:VAL:CG2	2.49	0.40
1:A:2233:VAL:HG12	1:A:2234:ARG:H	1.86	0.40
1:E:2131:LEU:CD2	1:E:2141:LEU:HD12	2.48	0.40
1:E:2243:GLN:HG2	1:E:2243:GLN:H	1.66	0.40
1:G:2137:GLU:OE2	1:G:2138:GLN:NE2	2.54	0.40
1:G:2315:ASP:H	1:G:2322:GLN:HE22	1.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	402/416 (97%)	369 (92%)	33 (8%)	0	100	100
1	C	380/416 (91%)	356 (94%)	24 (6%)	0	100	100
1	E	402/416 (97%)	375 (93%)	27 (7%)	0	100	100
1	G	380/416 (91%)	357 (94%)	23 (6%)	0	100	100
2	B	142/151 (94%)	134 (94%)	8 (6%)	0	100	100
2	D	129/151 (85%)	124 (96%)	5 (4%)	0	100	100
2	F	142/151 (94%)	136 (96%)	6 (4%)	0	100	100
2	H	135/151 (89%)	129 (96%)	6 (4%)	0	100	100
All	All	2112/2268 (93%)	1980 (94%)	132 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	347/351 (99%)	305 (88%)	42 (12%)	5	16
1	C	331/351 (94%)	294 (89%)	37 (11%)	6	18
1	E	347/351 (99%)	301 (87%)	46 (13%)	4	13
1	G	331/351 (94%)	302 (91%)	29 (9%)	9	28
2	B	123/117 (105%)	99 (80%)	24 (20%)	1	4
2	D	115/117 (98%)	99 (86%)	16 (14%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	123/117 (105%)	109 (89%)	14 (11%)	5	18
2	H	119/117 (102%)	104 (87%)	15 (13%)	4	14
All	All	1836/1872 (98%)	1613 (88%)	223 (12%)	5	16

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2003	ARG
1	A	2008	VAL
1	A	2009	SER
1	A	2033	LYS
1	A	2059	LEU
1	A	2062	LEU
1	A	2083	SER
1	A	2091	ARG
1	A	2104	VAL
1	A	2117	ILE
1	A	2125	ARG
1	A	2131	LEU
1	A	2138	GLN
1	A	2168	VAL
1	A	2177	ARG
1	A	2184	ASN
1	A	2191	ARG
1	A	2192	GLN
1	A	2203	ARG
1	A	2218	ASP
1	A	2222	ARG
1	A	2224	LEU
1	A	2231	VAL
1	A	2235	PHE
1	A	2238	LEU
1	A	2239	SER
1	A	2242	ARG
1	A	2243	GLN
1	A	2245	GLU
1	A	2247	LEU
1	A	2249	ASP
1	A	2250	ASN
1	A	2255	LYS
1	A	2266	LEU

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Mol	Chain	Res	Type
1	A	2269	ILE
1	A	2292	GLU
1	A	2315	ASP
1	A	2322	GLN
1	A	2350	LYS
1	A	2351	VAL
1	A	2358	ARG
1	A	2360	ARG
2	B	6	THR
2	B	18	SER
2	B	28	ILE
2	B	49	LEU
2	B	51	ASP
2	B	52	MSE
2	B	53	ILE
2	B	57	ASP
2	B	68	GLU
2	B	72	MSE
2	B	77	MSE
2	B	87	ARG
2	B	88	GLU
2	B	92	VAL
2	B	95	LYS
2	B	111	THR
2	B	115	GLU
2	B	117	LEU
2	B	120	GLU
2	B	121	GLU
2	B	126	ILE
2	B	132	ASP
2	B	139	TYR
2	B	145	MSE
1	C	1973	ARG
1	C	1976	LYS
1	C	2005	ASP
1	C	2030	GLN
1	C	2060	THR
1	C	2061	LYS
1	C	2088	LYS
1	C	2091	ARG
1	C	2093	ILE
1	C	2104	VAL

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Mol	Chain	Res	Type
1	C	2105	VAL
1	C	2118	ASP
1	C	2125	ARG
1	C	2130	PHE
1	C	2132	ASP
1	C	2139	ASN
1	C	2145	ILE
1	C	2150	PHE
1	C	2151	SER
1	C	2165	GLN
1	C	2176	VAL
1	C	2224	LEU
1	C	2231	VAL
1	C	2234	ARG
1	C	2260	VAL
1	C	2262	LEU
1	C	2269	ILE
1	C	2271	SER
1	C	2282	LEU
1	C	2284	THR
1	C	2289	LEU
1	C	2312	ILE
1	C	2315	ASP
1	C	2358	ARG
1	C	2361	ILE
1	C	2364	GLN
1	C	2371	THR
2	D	5	LEU
2	D	21	ASP
2	D	31	LYS
2	D	35	THR
2	D	65	ASP
2	D	70	LEU
2	D	71	THR
2	D	73	MSE
2	D	76	LYS
2	D	77	MSE
2	D	83	GLU
2	D	86	ILE
2	D	96	ASP
2	D	127	ARG
2	D	139	TYR

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Mol	Chain	Res	Type
2	D	145	MSE
1	E	1976	LYS
1	E	1990	VAL
1	E	2004	VAL
1	E	2011	GLU
1	E	2017	ILE
1	E	2018	GLN
1	E	2021	SER
1	E	2026	HIS
1	E	2030	GLN
1	E	2051	ASP
1	E	2060	THR
1	E	2073	HIS
1	E	2091	ARG
1	E	2108	ILE
1	E	2113	ASN
1	E	2118	ASP
1	E	2125	ARG
1	E	2130	PHE
1	E	2131	LEU
1	E	2135	ASN
1	E	2137	GLU
1	E	2140	GLN
1	E	2142	LYS
1	E	2152	ASN
1	E	2192	GLN
1	E	2201	GLU
1	E	2218	ASP
1	E	2222	ARG
1	E	2231	VAL
1	E	2235	PHE
1	E	2242	ARG
1	E	2243	GLN
1	E	2245	GLU
1	E	2255	LYS
1	E	2258	THR
1	E	2264	VAL
1	E	2266	LEU
1	E	2291	GLN
1	E	2295	GLU
1	E	2306	ASP
1	E	2308	LYS

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Mol	Chain	Res	Type
1	E	2309	SER
1	E	2347	VAL
1	E	2352	LEU
1	E	2355	HIS
1	E	2358	ARG
2	F	5	LEU
2	F	6	THR
2	F	8	GLU
2	F	23	ASP
2	F	25	ASP
2	F	38	ARG
2	F	64	ILE
2	F	68	GLU
2	F	76	LYS
2	F	107	ARG
2	F	117	LEU
2	F	121	GLU
2	F	132	ASP
2	F	146	MSE
1	G	1973	ARG
1	G	1988	ASN
1	G	1990	VAL
1	G	1994	LYS
1	G	2001	PHE
1	G	2014	GLN
1	G	2049	ASP
1	G	2073	HIS
1	G	2083	SER
1	G	2104	VAL
1	G	2129	LEU
1	G	2131	LEU
1	G	2137	GLU
1	G	2140	GLN
1	G	2152	ASN
1	G	2153	THR
1	G	2176	VAL
1	G	2184	ASN
1	G	2222	ARG
1	G	2235	PHE
1	G	2266	LEU
1	G	2281	SER
1	G	2286	ARG

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Mol	Chain	Res	Type
1	G	2300	ARG
1	G	2312	ILE
1	G	2326	ILE
1	G	2333	ASN
1	G	2337	PHE
1	G	2352	LEU
2	H	10	ILE
2	H	19	LEU
2	H	23	ASP
2	H	52	MSE
2	H	61	ASN
2	H	68	GLU
2	H	69	PHE
2	H	86	ILE
2	H	96	ASP
2	H	98	ASN
2	H	102	SER
2	H	110	MSE
2	H	111	THR
2	H	132	ASP
2	H	137	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2014	GLN
1	A	2018	GLN
1	A	2029	ASN
1	A	2073	HIS
1	A	2089	GLN
1	A	2098	GLN
1	A	2120	ASN
1	A	2138	GLN
1	A	2140	GLN
1	A	2152	ASN
1	A	2184	ASN
1	A	2243	GLN
1	A	2250	ASN
1	A	2287	ASN
1	A	2333	ASN
1	A	2349	ASN
1	A	2354	HIS

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Mol	Chain	Res	Type
1	A	2364	GLN
2	B	54	ASN
2	B	61	ASN
2	B	108	HIS
2	B	138	ASN
1	C	2018	GLN
1	C	2098	GLN
1	C	2120	ASN
1	C	2139	ASN
1	C	2166	ASN
1	C	2184	ASN
1	C	2192	GLN
1	C	2287	ASN
1	C	2316	ASN
1	C	2355	HIS
2	D	42	GLN
2	D	50	GLN
2	D	108	HIS
2	D	136	GLN
1	E	2098	GLN
1	E	2135	ASN
1	E	2138	GLN
1	E	2140	GLN
1	E	2219	GLN
1	E	2243	GLN
1	E	2339	GLN
1	E	2354	HIS
2	F	54	ASN
2	F	61	ASN
2	F	108	HIS
2	F	138	ASN
1	G	2096	ASN
1	G	2098	GLN
1	G	2120	ASN
1	G	2140	GLN
1	G	2152	ASN
1	G	2184	ASN
1	G	2192	GLN
1	G	2287	ASN
1	G	2322	GLN
1	G	2333	ASN
1	G	2349	ASN

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Mol	Chain	Res	Type
2	H	42	GLN
2	H	98	ASN
2	H	136	GLN
2	H	138	ASN

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	399/416 (95%)	0.73	54 (13%) 7 5	19, 51, 97, 123	0
1	C	379/416 (91%)	0.46	30 (7%) 18 13	17, 44, 86, 137	0
1	E	399/416 (95%)	0.55	37 (9%) 14 10	19, 42, 87, 113	0
1	G	379/416 (91%)	0.49	33 (8%) 16 11	15, 45, 87, 117	0
2	B	135/151 (89%)	1.04	21 (15%) 5 4	24, 67, 113, 129	0
2	D	124/151 (82%)	1.07	18 (14%) 6 4	32, 76, 103, 122	0
2	F	135/151 (89%)	0.70	13 (9%) 13 10	22, 49, 88, 122	0
2	H	130/151 (86%)	1.21	25 (19%) 3 2	28, 78, 115, 146	0
All	All	2080/2268 (91%)	0.67	231 (11%) 10 7	15, 50, 96, 146	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	5	LEU	5.7
2	H	5	LEU	5.4
1	C	2362	ILE	5.2
1	G	2073	HIS	5.0
1	A	2362	ILE	4.9
1	C	2131	LEU	4.6
1	A	2295	GLU	4.6
2	H	53	ILE	4.5
1	C	2370	TRP	4.5
1	C	2360	ARG	4.4
1	E	2252	ASP	4.4
1	G	2235	PHE	4.2
2	B	33	LEU	4.2
1	A	2029	ASN	4.1
1	A	2006	VAL	4.1
2	B	32	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	2137	GLU	4.0
2	F	5	LEU	4.0
1	A	2247	LEU	4.0
1	G	2131	LEU	3.9
2	D	89	ALA	3.8
1	G	2360	ARG	3.8
1	A	2248	ALA	3.8
1	G	2075	GLU	3.7
1	G	2362	ILE	3.7
1	A	2294	GLU	3.7
1	C	2130	PHE	3.7
2	B	64	ILE	3.7
1	A	2359	THR	3.6
1	C	2072	PRO	3.6
1	G	2129	LEU	3.6
1	G	2350	LYS	3.6
2	H	22	LYS	3.5
2	B	24	GLY	3.5
2	B	70	LEU	3.5
1	G	2358	ARG	3.4
2	B	56	VAL	3.4
1	G	2364	GLN	3.4
2	F	131	ILE	3.3
1	A	1987	ASP	3.3
1	A	2246	LEU	3.3
1	C	2235	PHE	3.3
2	B	69	PHE	3.3
1	C	2132	ASP	3.2
1	E	2249	ASP	3.2
1	A	2011	GLU	3.2
2	H	49	LEU	3.2
2	D	32	GLU	3.2
1	A	2369	ALA	3.2
1	E	2242	ARG	3.1
1	E	2246	LEU	3.1
2	B	19	LEU	3.1
1	A	2354	HIS	3.1
1	E	2086	ASN	3.1
1	G	2371	THR	3.1
1	A	2242	ARG	3.1
1	E	2294	GLU	3.1
1	C	2256	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	2074	ALA	3.0
1	E	2053	ASP	3.0
2	B	26	GLY	3.0
1	E	2362	ILE	3.0
2	D	81	ASP	3.0
1	A	2098	GLN	3.0
1	C	2358	ARG	2.9
1	A	2008	VAL	2.9
1	A	2093	ILE	2.9
2	B	71	THR	2.9
2	H	90	PHE	2.9
1	E	2326	ILE	2.9
2	H	139	TYR	2.9
1	E	2007	ASP	2.9
1	A	2252	ASP	2.9
1	A	2129	LEU	2.9
2	H	101	ILE	2.9
1	E	2300	ARG	2.8
1	A	2076	LYS	2.8
1	C	2129	LEU	2.8
2	H	71	THR	2.8
1	C	2133	PRO	2.8
1	A	2235	PHE	2.8
1	E	2248	ALA	2.8
1	A	2108	ILE	2.8
2	B	63	THR	2.8
2	H	15	GLU	2.7
1	E	2008	VAL	2.7
1	E	2130	PHE	2.7
1	A	2367	ASP	2.7
1	E	1968	SER	2.7
2	B	135	GLY	2.7
2	H	114	GLY	2.7
1	G	2361	ILE	2.7
1	E	2013	LYS	2.7
1	C	2071	ALA	2.7
2	H	63	THR	2.7
1	G	2306	ASP	2.7
1	A	2292	GLU	2.7
1	E	2030	GLN	2.7
2	H	30	THR	2.7
1	E	2136	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	71	THR	2.6
1	E	2237	ALA	2.6
2	D	148	ALA	2.6
2	D	79	ASP	2.6
1	E	2026	HIS	2.6
1	A	2251	PRO	2.6
1	A	2361	ILE	2.6
2	F	56	VAL	2.6
1	E	2366	GLU	2.6
1	C	1988	ASN	2.6
2	B	102	SER	2.5
1	A	2371	THR	2.5
1	C	2192	GLN	2.5
2	F	68	GLU	2.5
2	H	50	GLN	2.5
1	G	2218	ASP	2.5
2	D	102	SER	2.5
1	G	2266	LEU	2.5
2	F	124	GLN	2.5
1	C	2134	ASP	2.5
1	A	2238	LEU	2.5
2	F	70	LEU	2.5
2	D	95	LYS	2.5
1	C	2266	LEU	2.4
1	E	2367	ASP	2.4
1	A	2133	PRO	2.4
2	D	90	PHE	2.4
1	A	2030	GLN	2.4
1	G	2213	LYS	2.4
1	A	2086	ASN	2.4
2	F	49	LEU	2.4
1	A	2072	PRO	2.4
1	G	2134	ASP	2.4
1	A	2083	SER	2.4
1	A	2074	ALA	2.4
1	C	2136	ALA	2.4
2	H	100	TYR	2.4
1	E	2238	LEU	2.4
1	A	1988	ASN	2.4
2	B	28	ILE	2.4
1	C	2218	ASP	2.4
1	E	2307	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	2137	GLU	2.4
2	F	13	PHE	2.4
1	A	2071	ALA	2.4
2	B	148	ALA	2.4
2	H	23	ASP	2.4
1	E	2235	PHE	2.4
2	B	20	PHE	2.4
1	C	2075	GLU	2.4
2	D	139	TYR	2.4
1	C	2073	HIS	2.4
1	A	2250	ASN	2.3
2	B	133	GLY	2.3
1	E	2236	ASP	2.3
2	H	47	ALA	2.3
1	G	2219	GLN	2.3
1	G	2133	PRO	2.3
1	G	2128	GLY	2.3
1	C	2074	ALA	2.3
2	H	89	ALA	2.3
1	C	2219	GLN	2.3
2	B	131	ILE	2.3
1	G	2084	GLY	2.3
2	H	32	GLU	2.3
1	A	2138	GLN	2.3
1	A	2073	HIS	2.3
1	G	2233	VAL	2.3
1	A	2113	ASN	2.3
2	H	83	GLU	2.3
1	E	2010	ASP	2.3
1	E	2243	GLN	2.3
2	D	96	ASP	2.3
1	G	2027	THR	2.3
1	A	2366	GLU	2.2
1	E	2295	GLU	2.2
1	E	2247	LEU	2.2
2	D	28	ILE	2.2
2	B	27	THR	2.2
2	F	63	THR	2.2
1	A	2031	VAL	2.2
1	A	2233	VAL	2.2
2	B	21	ASP	2.2
1	A	2370	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	2370	TRP	2.2
1	A	2368	GLY	2.2
1	E	1994	LYS	2.2
1	G	2365	LYS	2.2
2	F	148	ALA	2.2
1	A	2136	ALA	2.2
1	G	2321	ALA	2.2
2	H	84	GLU	2.2
1	A	2018	GLN	2.2
1	G	2333	ASN	2.2
1	C	2306	ASP	2.2
1	G	2072	PRO	2.2
1	A	2128	GLY	2.2
1	A	2276	SER	2.2
1	C	2313	LEU	2.2
1	A	2227	ALA	2.2
1	E	2358	ARG	2.1
1	E	2360	ARG	2.1
2	D	132	ASP	2.1
2	F	30	THR	2.1
2	H	93	PHE	2.1
2	H	62	GLY	2.1
2	H	70	LEU	2.1
2	D	10	ILE	2.1
1	A	2364	GLN	2.1
1	E	2088	LYS	2.1
1	C	2367	ASP	2.1
2	D	135	GLY	2.1
1	A	2244	ALA	2.1
1	A	2212	TYR	2.1
1	E	2011	GLU	2.1
2	D	88	GLU	2.1
1	C	2233	VAL	2.1
2	H	76	LYS	2.1
1	G	2368	GLY	2.1
1	E	2073	HIS	2.0
1	G	2132	ASP	2.0
2	D	64	ILE	2.0
1	C	2363	ALA	2.0
1	G	2217	ALA	2.0
1	C	2308	LYS	2.0
2	H	92	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	53	ILE	2.0
2	F	29	THR	2.0
1	A	2010	ASP	2.0
2	D	105	GLU	2.0
1	E	2006	VAL	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
3	MG	F	201	1/1	0.88	0.15	27,27,27,27	0
3	MG	F	202	1/1	0.92	0.11	56,56,56,56	0
3	MG	F	203	1/1	0.96	0.18	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.