



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:34 PM UTC

PDB ID : 4I2V / pdb_00004i2v
Title : X-ray structure of the unliganded uridine phosphorylase from *Yersinia pseudotuberculosis* at 2.12Å resolution
Authors : Lashkov, A.A.; Balaev, V.V.; Prokofev, I.I.; Betzel, C.; Gabdoulkhakov, A.G.; Mikhailov, A.M.
Deposited on : 2012-11-23
Resolution : 2.12 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

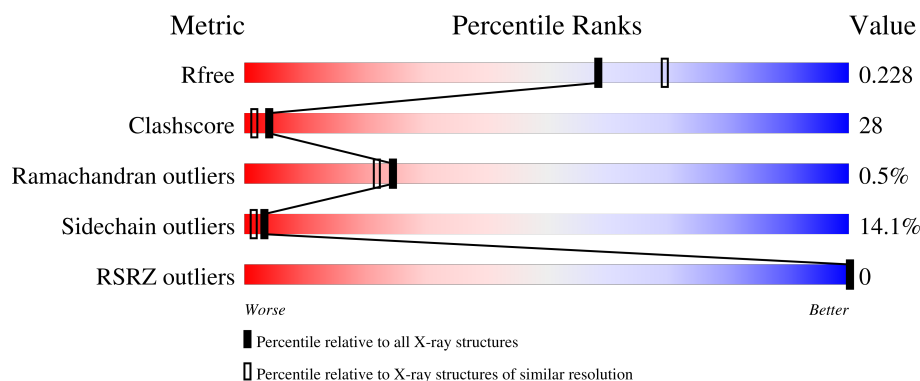
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	253	43% 49% 7%
1	B	253	45% 42% 12%
1	C	253	40% 48% 11%
1	D	253	40% 50% 8%
1	E	253	44% 45% 10%

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Mol	Chain	Length	Quality of chain
1	F	253	46% 47% 6% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11322 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			
1	B	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			
1	C	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			
1	D	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			
1	E	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			
1	F	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			

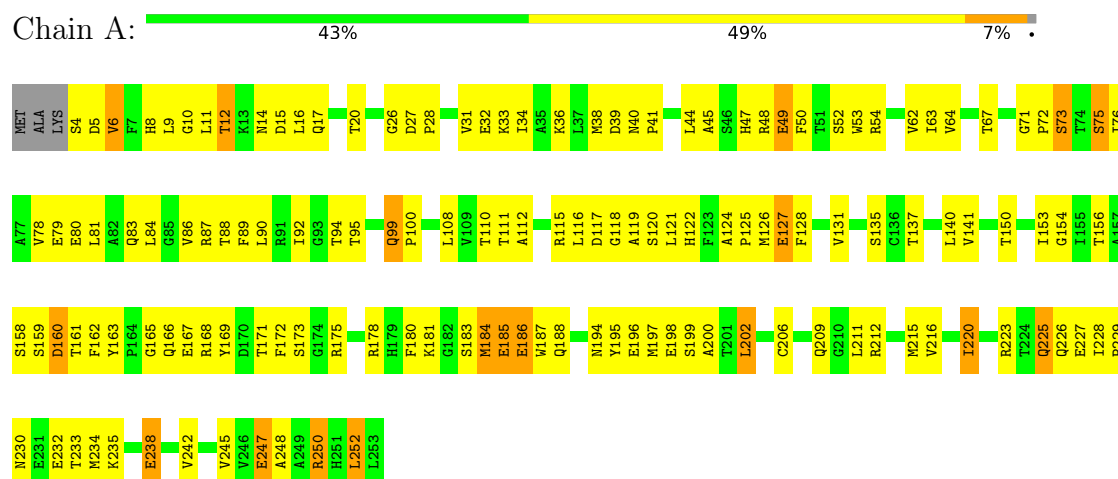
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	17	Total	O	0	0
			17	17		
2	C	13	Total	O	0	0
			13	13		
2	D	17	Total	O	0	0
			17	17		
2	E	4	Total	O	0	0
			4	4		
2	F	9	Total	O	0	0
			9	9		

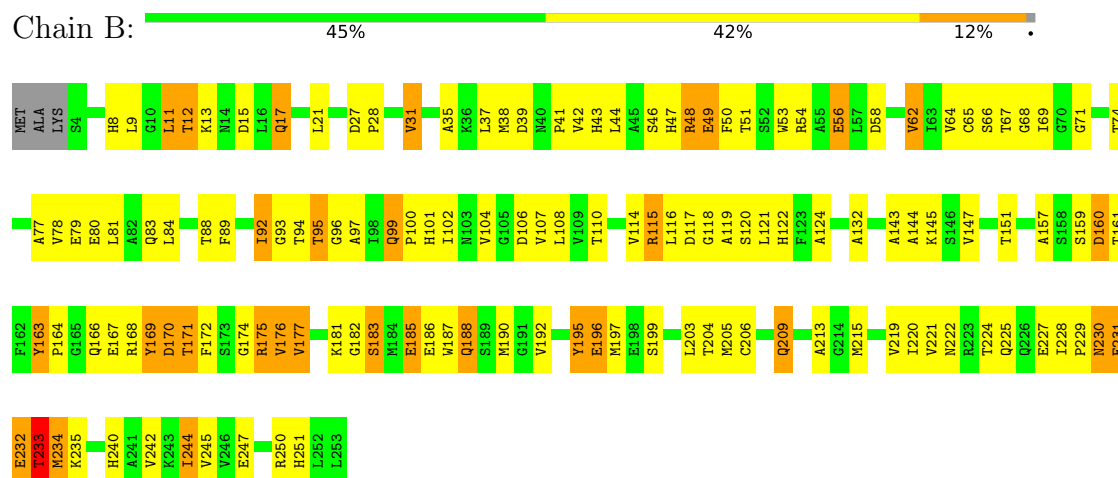
3 Residue-property plots

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: Uridine phosphorylase

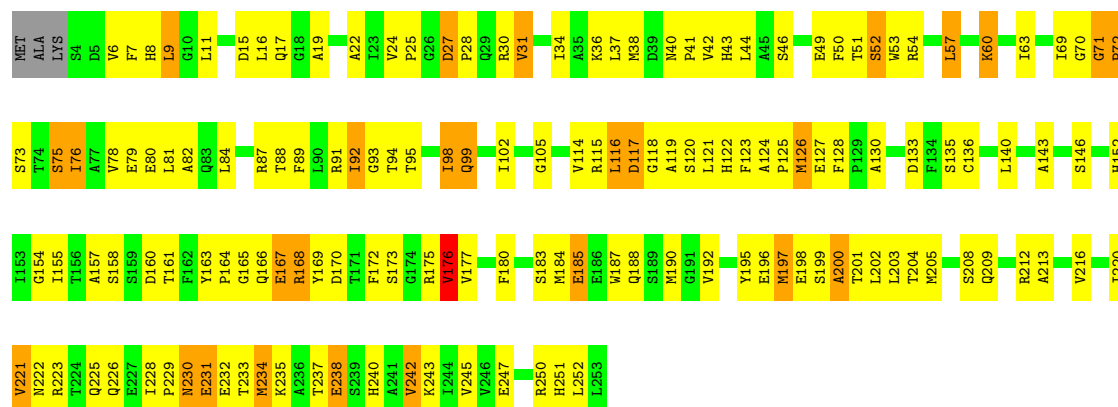


• Molecule 1: Uridine phosphorylase



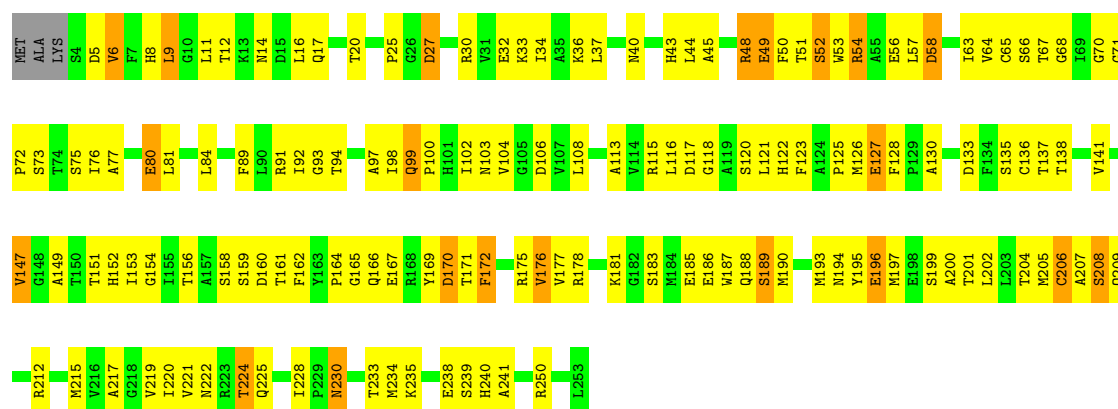
• Molecule 1: Uridine phosphorylase





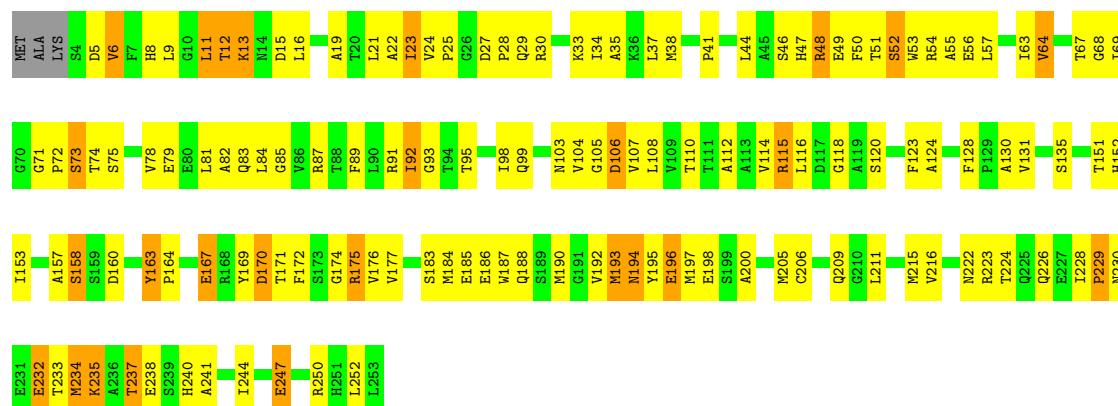
• Molecule 1: Uridine phosphorylase

Chain D: 40% 50% 8% .



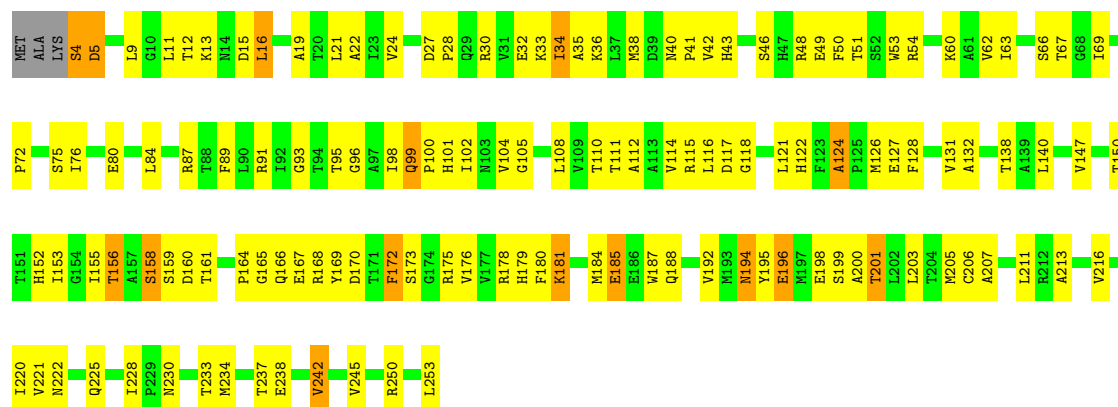
• Molecule 1: Uridine phosphorylase

Chain E: 44% 45% 10% .



• Molecule 1: Uridine phosphorylase

Chain F: 46% 47% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	156.68Å 156.68Å 48.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.61 – 2.12 29.61 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.61-2.12) 97.7 (29.61-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.200 , 0.242 0.202 , 0.228	Depositor DCC
R_{free} test set	3680 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 16.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.427 for -h,-k,l 0.075 for h,-h-k,-l 0.074 for -k,-h,-l	Xtriage
Reported twinning fraction	0.460 for -h,-k,l	Depositor
Outliers	0 of 73600 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11322	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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

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	0.60	0/1908	1.03	6/2590 (0.2%)
1	B	0.61	0/1908	1.11	12/2590 (0.5%)
1	C	0.59	0/1908	1.12	14/2590 (0.5%)
1	D	0.60	0/1908	1.04	7/2590 (0.3%)
1	E	0.55	0/1908	1.06	13/2590 (0.5%)
1	F	0.59	0/1908	1.05	9/2590 (0.3%)
All	All	0.59	0/11448	1.07	61/15540 (0.4%)

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	B	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	SER	N-CA-C	-8.64	101.81	111.14
1	C	71	GLY	CA-C-N	8.62	127.93	118.97
1	C	71	GLY	C-N-CA	8.62	127.93	118.97
1	F	124	ALA	CA-C-N	7.41	127.08	119.82
1	F	124	ALA	C-N-CA	7.41	127.08	119.82
1	B	99	GLN	CA-C-N	7.27	127.90	119.47
1	B	99	GLN	C-N-CA	7.27	127.90	119.47
1	A	209	GLN	N-CA-C	7.12	121.68	112.92
1	E	169	TYR	N-CA-C	-6.98	104.77	113.28
1	C	27	ASP	CA-C-N	6.76	127.02	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	27	ASP	C-N-CA	6.76	127.02	119.32
1	D	127	GLU	N-CA-C	-6.47	104.65	112.54
1	B	11	LEU	N-CA-C	6.33	119.09	110.55
1	C	200	ALA	N-CA-C	-6.32	104.08	110.97
1	B	169	TYR	N-CA-C	-6.26	105.22	112.92
1	A	99	GLN	CA-C-N	6.16	126.27	119.87
1	A	99	GLN	C-N-CA	6.16	126.27	119.87
1	C	121	LEU	N-CA-C	-6.11	105.79	113.18
1	E	115	ARG	N-CA-C	6.01	119.67	112.93
1	E	194	ASN	N-CA-C	6.01	118.20	109.07
1	F	194	ASN	N-CA-C	5.95	116.26	107.88
1	C	154	GLY	N-CA-C	5.92	117.87	110.29
1	C	99	GLN	CA-C-N	5.85	125.95	119.87
1	C	99	GLN	C-N-CA	5.85	125.95	119.87
1	B	163	TYR	CA-C-N	-5.76	113.83	119.64
1	B	163	TYR	C-N-CA	-5.76	113.83	119.64
1	F	127	GLU	N-CA-C	-5.74	105.77	112.89
1	B	233	THR	N-CA-C	5.69	122.91	110.80
1	B	48	ARG	CB-CA-C	-5.65	110.04	116.54
1	C	197	MET	N-CA-C	5.65	120.30	112.45
1	B	115	ARG	N-CA-C	5.52	119.12	112.93
1	E	228	ILE	CA-C-N	5.52	126.74	119.84
1	E	228	ILE	C-N-CA	5.52	126.74	119.84
1	B	31	VAL	CB-CA-C	-5.50	104.94	111.81
1	A	225	GLN	N-CA-C	5.47	118.49	109.85
1	E	163	TYR	CA-C-N	-5.45	114.14	119.64
1	E	163	TYR	C-N-CA	-5.45	114.14	119.64
1	D	49	GLU	CA-C-N	-5.38	114.51	122.41
1	D	49	GLU	C-N-CA	-5.38	114.51	122.41
1	B	163	TYR	N-CA-C	5.34	121.61	109.81
1	A	150	THR	N-CA-C	-5.33	99.82	108.41
1	E	232	GLU	N-CA-C	-5.33	99.84	108.41
1	E	68	GLY	N-CA-C	-5.31	104.90	111.70
1	D	99	GLN	CA-C-N	5.30	124.91	119.56
1	D	99	GLN	C-N-CA	5.30	124.91	119.56
1	E	99	GLN	CA-C-N	5.29	125.10	119.28
1	E	99	GLN	C-N-CA	5.29	125.10	119.28
1	E	71	GLY	N-CA-C	5.25	123.04	112.34
1	F	150	THR	N-CA-C	-5.22	100.58	108.67
1	F	34	ILE	N-CA-C	5.22	116.69	111.00
1	C	127	GLU	N-CA-C	5.20	118.09	111.69
1	A	197	MET	N-CA-C	5.20	119.71	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	ILE	N-CA-C	5.19	115.25	107.51
1	C	31	VAL	N-CA-C	5.16	115.38	110.42
1	C	251	HIS	N-CA-C	-5.15	106.68	113.17
1	F	95	THR	N-CA-C	5.14	117.06	108.99
1	F	99	GLN	CA-C-N	5.13	124.79	119.56
1	F	99	GLN	C-N-CA	5.13	124.79	119.56
1	E	198	GLU	N-CA-C	5.06	119.60	113.38
1	D	71	GLY	CA-C-N	5.04	124.48	119.24
1	D	71	GLY	C-N-CA	5.04	124.48	119.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	232	GLU	Peptide
1	E	232	GLU	Peptide

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	1875	0	1869	123	0
1	B	1875	0	1869	108	0
1	C	1875	0	1869	116	0
1	D	1875	0	1869	124	0
1	E	1875	0	1869	101	0
1	F	1875	0	1869	97	0
2	A	12	0	0	1	0
2	B	17	0	0	0	0
2	C	13	0	0	1	0
2	D	17	0	0	4	0
2	E	4	0	0	0	0
2	F	9	0	0	1	0
All	All	11322	0	11214	620	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 28.

All (620) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:HB3	1:B:164:PRO:HB2	1.43	1.00
1:F:16:LEU:HG	1:F:63:ILE:HG13	1.48	0.93
1:D:49:GLU:HG2	1:D:68:GLY:HA2	1.55	0.88
1:E:167:GLU:HG3	1:E:183:SER:HB2	1.54	0.87
1:E:164:PRO:HB2	1:F:122:HIS:HB3	1.57	0.85
1:A:8:HIS:CD2	1:A:50:PHE:HE2	1.95	0.83
1:E:175:ARG:HH21	1:E:177:VAL:HA	1.44	0.82
1:C:72:PRO:HG2	1:D:72:PRO:HD2	1.62	0.80
1:C:115:ARG:HH21	1:C:120:SER:HB2	1.46	0.79
1:C:49:GLU:HG3	1:D:49:GLU:HB2	1.64	0.79
1:E:229:PRO:HG2	1:E:234:MET:HE2	1.65	0.79
1:C:187:TRP:HB3	1:C:192:VAL:HB	1.65	0.79
1:A:8:HIS:HD2	1:A:50:PHE:HE2	1.32	0.78
1:C:94:THR:HB	1:C:220:ILE:HD13	1.64	0.78
1:A:8:HIS:CD2	1:A:50:PHE:CE2	2.70	0.78
1:A:8:HIS:HB3	1:A:50:PHE:CD2	2.19	0.78
1:C:199:SER:HA	1:C:202:LEU:HB3	1.67	0.76
1:C:175:ARG:NH2	1:D:123:PHE:O	2.20	0.75
1:A:8:HIS:HB3	1:A:50:PHE:CE2	2.22	0.75
1:D:65:CYS:HB3	1:D:81:LEU:HD11	1.68	0.74
1:B:102:ILE:O	1:B:222:ASN:ND2	2.21	0.74
1:E:16:LEU:HB3	1:E:19:ALA:HB3	1.70	0.73
1:B:99:GLN:HB3	1:B:101:HIS:CE1	2.23	0.73
1:B:99:GLN:NE2	1:B:188:GLN:O	2.21	0.73
1:A:99:GLN:NE2	1:A:188:GLN:O	2.22	0.72
1:A:185:GLU:HA	1:A:188:GLN:HB2	1.70	0.72
1:C:71:GLY:O	1:C:75:SER:N	2.23	0.72
1:F:196:GLU:OE2	1:F:199:SER:N	2.22	0.72
1:A:115:ARG:NH1	1:A:128:PHE:O	2.24	0.70
1:C:16:LEU:HD22	1:C:63:ILE:HG13	1.74	0.70
1:B:43:HIS:NE2	1:B:46:SER:OG	2.25	0.70
1:D:5:ASP:H	1:D:12:THR:HG22	1.58	0.69
1:D:222:ASN:HB3	1:D:225:GLN:HB2	1.74	0.69
1:C:17:GLN:HB3	1:C:54:ARG:HH12	1.57	0.69
1:B:183:SER:HA	1:B:186:GLU:HB3	1.73	0.68
1:C:164:PRO:HB2	1:D:122:HIS:HB3	1.75	0.68
1:A:115:ARG:NH2	1:A:124:ALA:O	2.25	0.68
1:A:183:SER:HA	1:A:186:GLU:HB2	1.75	0.68
1:E:114:VAL:HB	1:E:157:ALA:HA	1.76	0.68
1:D:97:ALA:O	1:D:222:ASN:ND2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:LEU:HD21	1:E:54:ARG:HB2	1.76	0.67
1:F:102:ILE:HG21	1:F:108:LEU:HD21	1.75	0.67
1:F:89:PHE:HE2	1:F:211:LEU:HD13	1.60	0.67
1:E:34:ILE:HB	1:E:64:VAL:HG11	1.77	0.67
1:E:6:VAL:HG21	1:E:9:LEU:HB2	1.75	0.67
1:B:247:GLU:OE2	1:B:251:HIS:NE2	2.24	0.66
1:E:41:PRO:HB2	1:E:53:TRP:HZ3	1.60	0.66
1:E:205:MET:O	1:E:209:GLN:NE2	2.26	0.66
1:B:118:GLY:N	1:B:160:ASP:OD2	2.28	0.66
1:C:118:GLY:H	1:C:160:ASP:HB2	1.61	0.66
1:A:12:THR:H	1:A:15:ASP:HB3	1.61	0.65
1:E:110:THR:HB	1:E:215:MET:HB3	1.78	0.65
1:F:155:ILE:HG22	1:F:192:VAL:HG22	1.79	0.65
1:F:121:LEU:HD21	1:F:126:MET:HE2	1.77	0.65
1:A:198:GLU:OE1	1:A:198:GLU:N	2.30	0.65
1:B:175:ARG:HH12	1:B:177:VAL:HA	1.62	0.65
1:E:46:SER:HA	1:E:51:THR:HA	1.77	0.65
1:C:187:TRP:HA	1:C:190:MET:HB3	1.79	0.65
1:C:81:LEU:HA	1:C:84:LEU:HD12	1.79	0.64
1:A:72:PRO:HB3	1:B:197:MET:HE1	1.79	0.64
1:D:147:VAL:HG12	1:D:149:ALA:H	1.63	0.64
1:E:209:GLN:HB3	1:F:172:PHE:CE2	2.33	0.64
1:A:166:GLN:OE1	1:A:168:ARG:NH2	2.31	0.64
1:D:75:SER:HA	1:D:205:MET:HE1	1.80	0.63
1:A:16:LEU:HD23	1:A:63:ILE:HG13	1.80	0.63
1:C:115:ARG:NH1	1:C:128:PHE:O	2.30	0.63
1:D:6:VAL:HG22	1:D:11:LEU:H	1.62	0.63
1:F:140:LEU:HD22	1:F:216:VAL:HB	1.80	0.63
1:B:97:ALA:HB1	1:B:102:ILE:HB	1.81	0.63
1:F:161:THR:HB	1:F:164:PRO:HD2	1.80	0.63
1:A:6:VAL:HG21	1:A:84:LEU:HD11	1.79	0.63
1:C:99:GLN:NE2	1:C:192:VAL:O	2.30	0.63
1:B:115:ARG:NH2	1:B:124:ALA:O	2.31	0.62
1:B:115:ARG:NH2	1:B:120:SER:O	2.33	0.62
1:E:41:PRO:HB2	1:E:53:TRP:CZ3	2.35	0.62
1:F:238:GLU:O	1:F:242:VAL:HB	1.99	0.62
1:E:171:THR:HG23	1:E:174:GLY:H	1.64	0.62
1:A:118:GLY:N	1:A:160:ASP:OD2	2.31	0.62
1:F:30:ARG:HG3	1:F:33:LYS:HD3	1.81	0.62
1:A:26:GLY:O	1:B:48:ARG:NH2	2.33	0.62
1:E:57:LEU:HD13	1:E:250:ARG:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:HIS:CB	1:A:50:PHE:CE2	2.84	0.61
1:D:196:GLU:OE2	1:D:199:SER:N	2.31	0.61
1:B:170:ASP:N	1:B:170:ASP:OD1	2.34	0.61
1:C:187:TRP:O	1:C:190:MET:N	2.34	0.61
1:D:141:VAL:HG22	1:D:153:ILE:HG12	1.82	0.61
1:B:119:ALA:N	1:B:160:ASP:OD2	2.34	0.60
1:A:9:LEU:HD12	1:A:84:LEU:HD12	1.82	0.60
1:B:21:LEU:HG	1:B:88:THR:HB	1.83	0.60
1:D:25:PRO:HB3	1:D:92:ILE:HG23	1.83	0.60
1:A:158:SER:HA	1:A:196:GLU:O	2.02	0.60
1:C:163:TYR:HB2	1:C:164:PRO:HD3	1.84	0.60
1:B:163:TYR:HB2	1:B:164:PRO:HD3	1.84	0.60
1:E:72:PRO:HG2	1:F:72:PRO:HD2	1.83	0.60
1:C:168:ARG:HD3	1:C:223:ARG:HH12	1.67	0.60
1:C:72:PRO:HG2	1:D:72:PRO:CD	2.32	0.59
1:F:32:GLU:HG2	1:F:36:LYS:HE2	1.84	0.59
1:A:72:PRO:HG3	1:B:160:ASP:O	2.02	0.59
1:C:91:ARG:HB2	1:C:202:LEU:HD21	1.84	0.59
1:D:115:ARG:HH21	1:D:120:SER:HB2	1.68	0.59
1:E:69:ILE:HG13	1:F:48:ARG:HD2	1.84	0.59
1:E:118:GLY:N	1:E:160:ASP:OD2	2.30	0.59
1:A:247:GLU:HB2	1:A:250:ARG:HH21	1.67	0.59
1:B:159:SER:HB3	1:B:166:GLN:HG2	1.84	0.59
1:B:205:MET:O	1:B:209:GLN:HB2	2.02	0.59
1:E:209:GLN:HG2	1:F:173:SER:HB3	1.84	0.59
1:E:247:GLU:O	1:E:250:ARG:HG2	2.03	0.59
1:D:104:VAL:HA	1:D:219:VAL:HG12	1.85	0.59
1:E:92:ILE:HD13	1:E:93:GLY:N	2.18	0.59
1:A:33:LYS:NZ	1:A:238:GLU:OE1	2.30	0.58
1:B:17:GLN:OE1	1:B:54:ARG:NH1	2.36	0.58
1:C:44:LEU:HB2	1:C:52:SER:HB2	1.85	0.58
1:D:178:ARG:HA	1:D:181:LYS:HE3	1.85	0.58
1:C:76:ILE:HD11	1:D:162:PHE:HB2	1.84	0.58
1:D:118:GLY:O	1:D:122:HIS:ND1	2.35	0.58
1:F:158:SER:HA	1:F:196:GLU:O	2.03	0.58
1:B:166:GLN:HA	1:B:195:TYR:CE1	2.39	0.57
1:A:28:PRO:HD2	1:B:48:ARG:HG2	1.86	0.57
1:E:187:TRP:O	1:E:192:VAL:N	2.37	0.57
1:D:33:LYS:HZ3	1:D:239:SER:HA	1.68	0.57
1:E:95:THR:HG21	1:E:194:ASN:HD22	1.70	0.57
1:D:44:LEU:HD11	1:D:54:ARG:HB2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:GLN:NE2	1:D:197:MET:HG2	2.20	0.56
1:B:79:GLU:O	1:B:83:GLN:HB2	2.05	0.56
1:E:27:ASP:OD1	1:E:27:ASP:N	2.38	0.56
1:F:5:ASP:N	1:F:5:ASP:OD1	2.37	0.56
1:C:99:GLN:O	1:C:222:ASN:ND2	2.36	0.56
1:E:186:GLU:O	1:E:190:MET:N	2.38	0.56
1:B:67:THR:HG22	1:B:77:ALA:HB3	1.87	0.56
1:C:72:PRO:HD2	1:D:72:PRO:HG2	1.87	0.56
1:F:111:THR:HG23	1:F:153:ILE:HG22	1.88	0.56
1:D:121:LEU:HD21	1:D:126:MET:HB2	1.87	0.56
1:A:122:HIS:ND1	1:B:161:THR:OG1	2.23	0.56
1:A:156:THR:OG1	1:A:194:ASN:OD1	2.21	0.56
1:E:13:LYS:HG2	1:E:84:LEU:HA	1.86	0.56
1:F:13:LYS:HA	1:F:84:LEU:HD22	1.87	0.56
1:E:49:GLU:OE2	1:F:69:ILE:N	2.37	0.56
1:E:115:ARG:NH2	1:E:124:ALA:O	2.25	0.56
1:D:233:THR:HG23	1:D:234:MET:H	1.70	0.56
1:A:45:ALA:HB1	1:A:47:HIS:CD2	2.41	0.56
1:A:115:ARG:HH21	1:A:121:LEU:HA	1.69	0.56
1:C:124:ALA:HB1	1:C:128:PHE:HB3	1.88	0.56
1:E:105:GLY:HA2	1:E:237:THR:HB	1.86	0.56
1:E:91:ARG:HG2	1:E:215:MET:SD	2.46	0.55
1:A:111:THR:HG23	1:A:153:ILE:HG22	1.89	0.55
1:B:114:VAL:HB	1:B:157:ALA:HA	1.88	0.55
1:C:221:VAL:HG23	1:C:229:PRO:HD3	1.89	0.55
1:A:80:GLU:HA	1:A:83:GLN:HB2	1.88	0.55
1:B:199:SER:HB3	1:B:215:MET:SD	2.46	0.55
1:A:49:GLU:HB2	1:B:49:GLU:HG3	1.88	0.55
1:A:95:THR:HG21	1:A:108:LEU:HD12	1.87	0.55
1:A:12:THR:HG23	1:A:15:ASP:HB2	1.89	0.55
1:A:206:CYS:HB3	1:A:211:LEU:O	2.06	0.55
1:B:118:GLY:HA2	1:B:121:LEU:HG	1.88	0.55
1:C:157:ALA:O	1:C:195:TYR:HA	2.07	0.55
1:E:108:LEU:HB3	1:E:193:MET:HE3	1.89	0.54
1:A:8:HIS:CG	1:A:50:PHE:CE2	2.95	0.54
1:F:98:ILE:O	1:F:188:GLN:HG2	2.08	0.54
1:B:247:GLU:O	1:B:250:ARG:HB3	2.08	0.54
1:C:118:GLY:HA3	1:D:118:GLY:HA3	1.88	0.54
1:C:242:VAL:HA	1:C:245:VAL:HG12	1.90	0.54
1:E:92:ILE:HG12	1:E:216:VAL:HG13	1.89	0.54
1:F:30:ARG:NH2	1:F:93:GLY:HA2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ALA:HA	1:B:38:MET:HE3	1.90	0.54
1:D:48:ARG:NH1	2:D:301:HOH:O	2.41	0.54
1:A:80:GLU:O	1:A:84:LEU:N	2.41	0.54
1:A:160:ASP:H	1:B:122:HIS:HE1	1.56	0.54
1:C:205:MET:O	1:C:209:GLN:HB2	2.07	0.54
1:A:33:LYS:NZ	1:A:238:GLU:HB3	2.23	0.53
1:B:74:THR:O	1:B:78:VAL:HG23	2.07	0.53
1:C:6:VAL:HG21	1:C:9:LEU:HB3	1.89	0.53
1:A:225:GLN:HG2	1:A:226:GLN:H	1.73	0.53
1:C:199:SER:O	1:C:203:LEU:N	2.22	0.53
1:D:196:GLU:CD	1:D:199:SER:H	2.16	0.53
1:D:158:SER:HA	1:D:196:GLU:O	2.08	0.53
1:B:12:THR:O	1:B:15:ASP:HB2	2.07	0.53
1:C:115:ARG:HB2	1:C:126:MET:SD	2.47	0.53
1:D:27:ASP:HB2	1:D:30:ARG:HG3	1.91	0.53
1:E:38:MET:HE3	1:E:55:ALA:HB3	1.90	0.53
1:F:206:CYS:O	1:F:211:LEU:N	2.34	0.53
1:C:198:GLU:OE2	1:C:198:GLU:N	2.40	0.53
1:D:67:THR:OG1	1:D:91:ARG:NH1	2.42	0.53
1:A:48:ARG:HG3	1:B:28:PRO:HD2	1.91	0.53
1:B:132:ALA:HA	1:B:203:LEU:HD22	1.90	0.53
1:D:16:LEU:HD13	1:D:84:LEU:HD13	1.91	0.53
1:A:16:LEU:HD11	1:A:84:LEU:HD13	1.89	0.53
1:A:116:LEU:HB2	1:A:159:SER:HA	1.91	0.53
1:A:88:THR:OG1	1:A:212:ARG:NH2	2.40	0.53
1:A:122:HIS:HB3	1:B:164:PRO:CB	2.26	0.53
1:E:206:CYS:HA	1:E:211:LEU:HD12	1.90	0.53
1:C:140:LEU:HD22	1:C:216:VAL:HB	1.90	0.52
1:F:233:THR:HG23	1:F:234:MET:H	1.74	0.52
1:C:28:PRO:HB3	1:C:51:THR:OG1	2.09	0.52
1:F:41:PRO:HB2	1:F:53:TRP:HZ3	1.74	0.52
1:E:112:ALA:HA	1:E:131:VAL:HA	1.90	0.52
1:A:112:ALA:HB2	1:A:131:VAL:HG23	1.91	0.52
1:A:184:MET:HE1	1:A:223:ARG:HB3	1.91	0.52
1:D:8:HIS:CD2	1:D:76:ILE:HD13	2.43	0.52
1:C:16:LEU:HB3	1:C:19:ALA:HB3	1.91	0.52
1:C:161:THR:CG2	1:C:164:PRO:HD2	2.40	0.52
1:D:30:ARG:NH1	1:D:94:THR:OG1	2.43	0.52
1:B:41:PRO:HB2	1:B:53:TRP:CZ3	2.45	0.52
1:F:67:THR:OG1	1:F:91:ARG:NH1	2.35	0.52
1:F:124:ALA:HB1	1:F:128:PHE:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:GLU:OE2	1:F:198:GLU:N	2.43	0.52
1:B:13:LYS:HZ2	1:B:84:LEU:HA	1.75	0.52
1:B:185:GLU:HA	1:B:188:GLN:HB3	1.90	0.52
1:C:114:VAL:HB	1:C:157:ALA:HA	1.92	0.52
1:D:92:ILE:HD11	1:D:241:ALA:HB1	1.91	0.52
1:D:97:ALA:HA	1:D:194:ASN:HA	1.92	0.52
1:D:115:ARG:HE	1:D:120:SER:HB2	1.73	0.52
1:F:184:MET:HE3	1:F:188:GLN:HE22	1.75	0.52
1:B:67:THR:HB	1:B:74:THR:HA	1.91	0.51
1:D:98:ILE:N	1:D:193:MET:O	2.39	0.51
1:B:116:LEU:HD21	1:B:187:TRP:HZ2	1.76	0.51
1:F:99:GLN:OE1	1:F:100:PRO:HD2	2.10	0.51
1:C:115:ARG:NH1	1:C:125:PRO:O	2.42	0.51
1:D:49:GLU:O	1:D:66:SER:OG	2.24	0.51
1:F:222:ASN:HB3	1:F:225:GLN:HB2	1.91	0.51
1:C:44:LEU:HD11	1:C:63:ILE:HD12	1.92	0.51
1:D:204:THR:O	1:D:208:SER:OG	2.27	0.51
1:E:29:GLN:O	1:E:33:LYS:HE2	2.10	0.51
1:F:76:ILE:O	1:F:80:GLU:HB2	2.09	0.51
1:A:33:LYS:HZ1	1:A:238:GLU:HB3	1.76	0.51
1:C:204:THR:O	1:C:208:SER:OG	2.28	0.51
1:D:108:LEU:HD22	1:D:152:HIS:HB2	1.93	0.51
1:C:230:ASN:OD1	1:C:230:ASN:N	2.44	0.51
1:D:117:ASP:HB2	1:D:160:ASP:OD1	2.11	0.51
1:D:147:VAL:HG12	1:D:149:ALA:N	2.25	0.51
1:C:167:GLU:HG2	1:C:176:VAL:HG11	1.91	0.51
1:A:41:PRO:HB2	1:A:53:TRP:CZ3	2.46	0.51
1:D:16:LEU:HG	1:D:63:ILE:HG13	1.91	0.51
1:D:185:GLU:HA	1:D:188:GLN:OE1	2.11	0.50
1:E:11:LEU:HD13	1:E:84:LEU:HD11	1.92	0.50
1:C:122:HIS:HB3	1:D:164:PRO:HG2	1.92	0.50
1:D:158:SER:HB2	1:D:196:GLU:OE2	2.12	0.50
1:E:9:LEU:HD11	1:E:81:LEU:HG	1.94	0.50
1:C:43:HIS:HB2	1:C:53:TRP:CE2	2.46	0.50
1:B:169:TYR:OH	1:B:181:LYS:HG3	2.12	0.50
1:E:234:MET:SD	1:E:234:MET:N	2.84	0.50
1:A:117:ASP:HA	1:A:160:ASP:HB2	1.94	0.50
1:A:162:PHE:O	1:A:166:GLN:HB2	2.11	0.50
1:C:79:GLU:HB2	1:C:205:MET:HE1	1.94	0.50
1:C:114:VAL:HG12	1:C:116:LEU:HG	1.93	0.50
1:F:99:GLN:HG2	1:F:192:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:MET:O	1:A:41:PRO:HG3	2.12	0.50
1:C:27:ASP:OD1	1:C:30:ARG:HB2	2.11	0.50
1:A:115:ARG:CZ	1:A:126:MET:HA	2.42	0.50
1:A:230:ASN:ND2	1:A:232:GLU:HB2	2.27	0.50
1:B:49:GLU:HG2	1:B:68:GLY:HA2	1.94	0.50
1:B:97:ALA:HB3	1:B:222:ASN:HD22	1.77	0.50
1:B:187:TRP:HB3	1:B:192:VAL:HB	1.94	0.49
1:F:110:THR:HG21	1:F:156:THR:HB	1.94	0.49
1:D:166:GLN:HE21	1:D:197:MET:HG2	1.77	0.49
1:E:24:VAL:O	1:E:91:ARG:HD2	2.12	0.49
1:E:163:TYR:HB2	1:E:164:PRO:HD3	1.93	0.49
1:A:4:SER:HB2	1:A:10:GLY:HA2	1.94	0.49
1:B:196:GLU:HG2	1:B:215:MET:HE1	1.93	0.49
1:D:11:LEU:HD21	1:D:44:LEU:HB3	1.94	0.49
1:F:43:HIS:HB2	1:F:53:TRP:CE2	2.47	0.49
1:C:11:LEU:HD21	1:C:52:SER:OG	2.13	0.49
1:C:78:VAL:O	1:C:82:ALA:N	2.36	0.49
1:C:173:SER:HB2	1:D:209:GLN:OE1	2.12	0.49
1:E:92:ILE:HD13	1:E:93:GLY:H	1.76	0.49
1:F:98:ILE:HD12	1:F:188:GLN:HG3	1.93	0.49
1:A:14:ASN:C	1:A:17:GLN:H	2.19	0.49
1:D:117:ASP:HB2	1:D:160:ASP:CG	2.37	0.49
1:E:106:ASP:HB3	1:E:152:HIS:NE2	2.28	0.49
1:F:42:VAL:O	1:F:54:ARG:N	2.41	0.49
1:B:50:PHE:CE1	1:B:77:ALA:HB2	2.48	0.49
1:C:196:GLU:CD	1:C:199:SER:H	2.20	0.49
1:D:89:PHE:N	1:D:212:ARG:O	2.43	0.49
1:E:157:ALA:N	1:E:194:ASN:O	2.45	0.49
1:E:197:MET:CE	1:F:72:PRO:HB3	2.42	0.49
1:C:31:VAL:HG12	1:C:53:TRP:HB2	1.95	0.49
1:A:122:HIS:CB	1:B:164:PRO:HB2	2.30	0.49
1:B:49:GLU:HG2	1:B:68:GLY:CA	2.41	0.49
1:D:68:GLY:HA3	1:D:73:SER:OG	2.13	0.49
1:F:36:LYS:NZ	2:F:308:HOH:O	2.45	0.49
1:A:87:ARG:HA	1:A:211:LEU:HD22	1.94	0.49
1:A:158:SER:HB3	1:A:200:ALA:HB2	1.95	0.49
1:F:30:ARG:HH22	1:F:93:GLY:HA2	1.76	0.49
1:A:6:VAL:HG11	1:A:80:GLU:HB3	1.94	0.48
1:A:199:SER:O	1:A:202:LEU:N	2.46	0.48
1:A:71:GLY:O	1:A:75:SER:N	2.34	0.48
1:B:114:VAL:HG12	1:B:116:LEU:HG	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:THR:H	1:A:15:ASP:CB	2.24	0.48
1:D:9:LEU:HB2	1:D:11:LEU:HD12	1.94	0.48
1:B:164:PRO:HA	1:B:176:VAL:HG22	1.94	0.48
1:C:117:ASP:OD1	1:C:120:SER:OG	2.29	0.48
1:E:187:TRP:HB3	1:E:192:VAL:HB	1.95	0.48
1:A:75:SER:O	1:A:79:GLU:N	2.29	0.48
1:A:125:PRO:O	1:A:127:GLU:N	2.40	0.48
1:F:132:ALA:HA	1:F:203:LEU:HD22	1.95	0.48
1:B:41:PRO:HB2	1:B:53:TRP:HZ3	1.78	0.48
1:E:104:VAL:HG11	1:E:229:PRO:HB3	1.96	0.48
1:E:230:ASN:OD1	1:E:230:ASN:N	2.46	0.48
1:F:115:ARG:NH1	1:F:128:PHE:O	2.45	0.48
1:A:158:SER:HB2	1:A:196:GLU:OE2	2.14	0.48
1:D:32:GLU:O	1:D:36:LYS:HG3	2.13	0.48
1:E:103:ASN:HB2	1:E:106:ASP:OD1	2.13	0.48
1:F:49:GLU:O	1:F:66:SER:OG	2.32	0.48
1:F:206:CYS:HB3	1:F:211:LEU:O	2.13	0.48
1:A:78:VAL:HG13	1:A:89:PHE:CZ	2.49	0.48
1:B:240:HIS:O	1:B:244:ILE:HD12	2.13	0.48
1:C:88:THR:OG1	1:C:212:ARG:NH2	2.46	0.48
1:C:240:HIS:O	1:C:243:LYS:HB3	2.14	0.48
1:D:54:ARG:NH2	1:D:56:GLU:HG3	2.29	0.48
1:D:186:GLU:O	1:D:190:MET:HG3	2.13	0.48
1:E:41:PRO:HA	1:E:54:ARG:O	2.13	0.48
1:E:72:PRO:HD2	1:F:72:PRO:HG2	1.96	0.48
1:B:224:THR:OG1	1:B:225:GLN:N	2.46	0.47
1:B:41:PRO:HA	1:B:54:ARG:O	2.14	0.47
1:E:75:SER:HB2	1:E:123:PHE:HZ	1.79	0.47
1:E:157:ALA:O	1:E:195:TYR:HA	2.14	0.47
1:D:48:ARG:N	1:D:48:ARG:HD3	2.29	0.47
1:F:96:GLY:O	1:F:194:ASN:HB2	2.14	0.47
1:A:6:VAL:HG23	1:A:11:LEU:H	1.79	0.47
1:B:230:ASN:OD1	1:B:230:ASN:N	2.47	0.47
1:C:25:PRO:HG3	1:C:34:ILE:HD12	1.96	0.47
1:C:158:SER:HA	1:C:196:GLU:O	2.15	0.47
1:E:28:PRO:HB3	1:E:51:THR:HB	1.95	0.47
1:C:98:ILE:HG21	1:C:195:TYR:CE2	2.50	0.47
1:F:4:SER:O	1:F:4:SER:OG	2.24	0.47
1:F:40:ASN:N	1:F:41:PRO:HD3	2.30	0.47
1:A:67:THR:O	1:A:73:SER:HB2	2.14	0.47
1:D:115:ARG:HG2	1:D:200:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:SER:HB3	1:D:215:MET:SD	2.55	0.47
1:E:8:HIS:HB3	1:E:50:PHE:HE2	1.80	0.47
1:E:16:LEU:HB3	1:E:19:ALA:CB	2.39	0.47
1:F:60:LYS:HB2	1:F:253:LEU:HD13	1.96	0.47
1:F:233:THR:HG23	1:F:234:MET:N	2.29	0.47
1:C:95:THR:O	1:C:220:ILE:HG12	2.15	0.47
1:A:248:ALA:O	1:A:252:LEU:HD12	2.15	0.47
1:C:28:PRO:HA	1:C:51:THR:HB	1.97	0.47
1:E:79:GLU:O	1:E:82:ALA:HB3	2.14	0.47
1:E:115:ARG:NH1	1:E:128:PHE:O	2.47	0.47
1:A:161:THR:OG1	1:B:122:HIS:ND1	2.27	0.47
1:F:99:GLN:HB3	1:F:101:HIS:CE1	2.50	0.47
1:B:167:GLU:OE2	1:B:183:SER:N	2.48	0.46
1:B:231:GLU:H	1:B:231:GLU:HG3	1.37	0.46
1:C:7:PHE:CD2	1:D:162:PHE:HE2	2.33	0.46
1:C:116:LEU:HD21	1:C:187:TRP:CZ2	2.50	0.46
1:C:116:LEU:HD12	1:C:157:ALA:HB1	1.96	0.46
1:D:30:ARG:O	1:D:34:ILE:HG12	2.15	0.46
1:A:17:GLN:HG3	1:A:54:ARG:NH1	2.31	0.46
1:C:60:LYS:HE3	1:C:60:LYS:H	1.79	0.46
1:C:234:MET:HA	2:C:312:HOH:O	2.15	0.46
1:A:187:TRP:CD1	1:A:195:TYR:HH	2.33	0.46
1:B:163:TYR:HA	1:B:168:ARG:HB2	1.97	0.46
1:B:196:GLU:OE2	1:B:199:SER:OG	2.23	0.46
1:C:228:ILE:HG22	1:C:229:PRO:O	2.15	0.46
1:F:112:ALA:HA	1:F:131:VAL:HA	1.98	0.46
1:B:233:THR:HG23	1:B:234:MET:N	2.30	0.46
1:C:119:ALA:O	1:C:122:HIS:HB2	2.15	0.46
1:E:222:ASN:OD1	1:E:224:THR:OG1	2.29	0.46
1:B:230:ASN:ND2	1:B:232:GLU:O	2.48	0.46
1:D:91:ARG:NH2	2:D:302:HOH:O	2.48	0.46
1:E:57:LEU:HD23	1:E:57:LEU:HA	1.73	0.46
1:F:16:LEU:HD23	1:F:19:ALA:N	2.31	0.46
1:A:167:GLU:HG2	1:A:169:TYR:CE2	2.51	0.46
1:F:9:LEU:HD11	1:F:80:GLU:HB3	1.98	0.46
1:A:14:ASN:O	1:A:17:GLN:HG2	2.15	0.46
1:C:38:MET:SD	1:C:57:LEU:HG	2.56	0.46
1:C:72:PRO:HB3	1:D:70:GLY:HA3	1.98	0.46
1:E:30:ARG:HG2	1:E:34:ILE:HD11	1.97	0.46
1:C:15:ASP:HB3	1:C:44:LEU:HD22	1.98	0.46
1:E:120:SER:HB3	1:E:200:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:LEU:HB2	1:F:159:SER:HA	1.98	0.46
1:A:78:VAL:HG13	1:A:89:PHE:CE2	2.51	0.45
1:B:15:ASP:O	1:B:54:ARG:NH1	2.48	0.45
1:C:36:LYS:HA	1:C:41:PRO:HG3	1.97	0.45
1:F:54:ARG:HA	1:F:63:ILE:HD13	1.98	0.45
1:C:168:ARG:NH1	1:C:170:ASP:OD2	2.49	0.45
1:E:241:ALA:HA	1:E:244:ILE:HD12	1.98	0.45
1:F:104:VAL:HG13	1:F:220:ILE:HA	1.98	0.45
1:A:90:LEU:HD11	1:A:252:LEU:HD13	1.97	0.45
1:B:171:THR:HG23	1:B:174:GLY:H	1.81	0.45
1:F:122:HIS:N	1:F:122:HIS:CD2	2.84	0.45
1:F:167:GLU:HG2	1:F:169:TYR:CE2	2.51	0.45
1:F:168:ARG:HH11	1:F:168:ARG:HB3	1.82	0.45
1:C:222:ASN:HB3	1:C:225:GLN:HB2	1.99	0.45
1:D:6:VAL:CG2	1:D:11:LEU:H	2.27	0.45
1:D:156:THR:HG23	1:D:194:ASN:ND2	2.32	0.45
1:A:41:PRO:HA	1:A:54:ARG:O	2.16	0.45
1:A:75:SER:OG	1:A:76:ILE:N	2.48	0.45
1:A:163:TYR:CD1	1:A:168:ARG:HD2	2.52	0.45
1:B:38:MET:SD	1:B:62:VAL:HG11	2.57	0.45
1:C:247:GLU:O	1:C:250:ARG:HG2	2.16	0.45
1:D:233:THR:HA	2:D:310:HOH:O	2.16	0.45
1:A:117:ASP:HB2	1:A:119:ALA:H	1.81	0.45
1:F:12:THR:OG1	1:F:15:ASP:OD1	2.34	0.45
1:F:46:SER:HA	1:F:51:THR:HA	1.98	0.45
1:A:125:PRO:C	1:A:127:GLU:H	2.23	0.45
1:E:79:GLU:O	1:E:83:GLN:HG3	2.17	0.45
1:E:158:SER:HA	1:E:196:GLU:O	2.16	0.45
1:F:16:LEU:HD22	1:F:84:LEU:O	2.17	0.45
1:B:92:ILE:HD13	1:B:93:GLY:N	2.31	0.45
1:A:140:LEU:HD22	1:A:216:VAL:HB	1.99	0.45
1:C:70:GLY:HA2	1:C:197:MET:HB3	1.99	0.45
1:D:201:THR:HG22	1:D:205:MET:SD	2.57	0.45
1:D:202:LEU:O	1:D:206:CYS:HB2	2.16	0.45
1:E:49:GLU:OE2	1:F:49:GLU:HG3	2.17	0.45
1:E:107:VAL:HB	1:E:151:THR:HG23	1.99	0.45
1:B:107:VAL:O	1:B:108:LEU:HD23	2.16	0.44
1:B:233:THR:HG23	1:B:235:LYS:H	1.81	0.44
1:D:169:TYR:CE1	1:D:176:VAL:HB	2.52	0.44
1:D:183:SER:O	1:D:187:TRP:NE1	2.50	0.44
1:F:89:PHE:O	1:F:213:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:GLN:HA	1:F:100:PRO:HD2	1.83	0.44
1:B:115:ARG:HH21	1:B:120:SER:C	2.25	0.44
1:B:167:GLU:OE1	1:B:182:GLY:N	2.31	0.44
1:C:40:ASN:O	1:C:42:VAL:HG23	2.18	0.44
1:C:183:SER:O	1:C:187:TRP:NE1	2.51	0.44
1:E:104:VAL:HG11	1:E:229:PRO:CB	2.47	0.44
1:E:196:GLU:HG2	1:E:215:MET:HE1	2.00	0.44
1:F:201:THR:O	1:F:205:MET:HG2	2.17	0.44
1:A:76:ILE:HA	1:B:163:TYR:HE2	1.83	0.44
1:B:65:CYS:HB3	1:B:81:LEU:HD11	1.99	0.44
1:B:116:LEU:HD21	1:B:187:TRP:CZ2	2.51	0.44
1:C:235:LYS:HA	1:C:238:GLU:HB3	1.99	0.44
1:F:179:HIS:HD2	1:F:180:PHE:CE1	2.35	0.44
1:A:28:PRO:HD3	1:A:49:GLU:OE2	2.18	0.44
1:D:137:THR:O	1:D:141:VAL:HG23	2.17	0.44
1:E:98:ILE:HG22	1:E:223:ARG:HD3	1.98	0.44
1:E:163:TYR:HB3	1:E:171:THR:HB	2.00	0.44
1:F:28:PRO:HD3	1:F:49:GLU:OE2	2.17	0.44
1:F:158:SER:HB2	1:F:200:ALA:HB2	1.98	0.44
1:C:128:PHE:CZ	1:C:208:SER:HB3	2.52	0.44
1:D:186:GLU:O	1:D:189:SER:OG	2.35	0.44
1:E:116:LEU:HD12	1:E:195:TYR:HE1	1.82	0.44
1:F:102:ILE:HG23	1:F:152:HIS:CD2	2.52	0.44
1:A:88:THR:HG21	1:A:252:LEU:HD22	1.99	0.44
1:C:114:VAL:HG23	1:C:155:ILE:HG22	2.00	0.44
1:D:115:ARG:NH1	1:D:128:PHE:O	2.50	0.44
1:A:83:GLN:HG2	1:B:172:PHE:CG	2.53	0.44
1:D:91:ARG:HG3	1:D:92:ILE:N	2.33	0.44
1:D:230:ASN:O	1:D:233:THR:HG22	2.18	0.44
1:E:22:ALA:HB3	1:E:89:PHE:CD1	2.53	0.44
1:A:137:THR:O	1:A:141:VAL:HG23	2.18	0.44
1:C:160:ASP:O	1:D:72:PRO:HG3	2.18	0.44
1:C:187:TRP:HB3	1:C:192:VAL:CB	2.43	0.44
1:D:6:VAL:HG22	1:D:11:LEU:O	2.18	0.44
1:B:81:LEU:HD13	1:B:89:PHE:HE1	1.83	0.43
1:B:104:VAL:HG11	1:B:229:PRO:HB3	2.00	0.43
1:C:133:ASP:HB3	1:C:136:CYS:HB2	2.00	0.43
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.79	0.43
1:E:69:ILE:HD12	1:F:50:PHE:HE1	1.81	0.43
1:F:87:ARG:H	1:F:87:ARG:HG2	1.62	0.43
1:F:184:MET:HE3	1:F:188:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HB3	1:A:86:VAL:HG21	2.00	0.43
1:A:122:HIS:CE1	1:B:161:THR:HG1	2.25	0.43
1:C:87:ARG:HD3	1:C:87:ARG:HA	1.79	0.43
1:C:209:GLN:HB3	1:D:172:PHE:CZ	2.53	0.43
1:D:97:ALA:HB3	1:D:222:ASN:HD22	1.83	0.43
1:A:8:HIS:CE1	1:A:76:ILE:HD13	2.53	0.43
1:B:144:ALA:HA	1:B:244:ILE:HG12	1.99	0.43
1:C:72:PRO:HG3	1:D:160:ASP:O	2.18	0.43
1:D:116:LEU:HB2	1:D:159:SER:HB3	2.01	0.43
1:E:205:MET:O	1:E:209:GLN:HB2	2.17	0.43
1:F:35:ALA:HA	1:F:38:MET:HE3	2.01	0.43
1:A:166:GLN:HG2	1:A:195:TYR:CD1	2.53	0.43
1:A:184:MET:O	1:A:188:GLN:HG3	2.18	0.43
1:C:102:ILE:HG12	1:C:152:HIS:CE1	2.53	0.43
1:D:40:ASN:HB3	1:D:54:ARG:HH22	1.84	0.43
1:A:242:VAL:O	1:A:245:VAL:HG12	2.18	0.43
1:B:11:LEU:HD21	1:B:44:LEU:HB3	2.00	0.43
1:B:100:PRO:O	1:B:225:GLN:NE2	2.51	0.43
1:B:169:TYR:CE2	1:B:176:VAL:HB	2.53	0.43
1:D:201:THR:O	1:D:205:MET:HG2	2.18	0.43
1:E:23:ILE:HG22	1:E:25:PRO:HD3	1.99	0.43
1:C:158:SER:OG	1:C:196:GLU:OE2	2.23	0.43
1:C:231:GLU:HG3	1:C:232:GLU:N	2.34	0.43
1:D:11:LEU:HD11	1:D:52:SER:OG	2.19	0.43
1:E:30:ARG:O	1:E:34:ILE:HG13	2.19	0.43
1:F:166:GLN:HA	1:F:195:TYR:CZ	2.52	0.43
1:A:34:ILE:CD1	1:A:92:ILE:HG21	2.49	0.43
1:D:43:HIS:HB2	1:D:53:TRP:CE2	2.54	0.43
1:D:170:ASP:OD1	1:D:170:ASP:N	2.50	0.43
1:A:6:VAL:CG2	1:A:11:LEU:H	2.32	0.43
1:A:94:THR:HB	1:A:220:ILE:HG12	1.99	0.43
1:B:94:THR:HB	1:B:220:ILE:HG23	2.00	0.43
1:B:190:MET:HB2	1:B:190:MET:HE3	1.78	0.43
1:B:206:CYS:SG	1:B:213:ALA:HB2	2.59	0.43
1:D:44:LEU:HD23	1:D:44:LEU:HA	1.91	0.43
1:D:91:ARG:HG2	1:D:215:MET:HG3	2.01	0.43
1:F:21:LEU:HD23	1:F:22:ALA:N	2.34	0.43
1:F:230:ASN:O	1:F:233:THR:HG22	2.18	0.43
1:A:20:THR:O	1:A:87:ARG:N	2.50	0.43
1:A:32:GLU:O	1:A:36:LYS:HG3	2.18	0.43
1:A:87:ARG:O	1:A:211:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HA	1:A:229:PRO:HD3	1.90	0.43
1:E:235:LYS:O	1:E:238:GLU:HB3	2.19	0.43
1:B:51:THR:N	1:B:66:SER:OG	2.50	0.43
1:C:123:PHE:O	1:D:175:ARG:NH2	2.48	0.43
1:D:133:ASP:HB3	1:D:136:CYS:HB2	2.01	0.43
1:E:234:MET:HA	1:E:237:THR:HG23	2.00	0.43
1:B:95:THR:O	1:B:220:ILE:HG12	2.18	0.42
1:C:70:GLY:HA3	1:D:72:PRO:HB2	2.01	0.42
1:C:118:GLY:N	1:C:160:ASP:HB2	2.32	0.42
1:A:233:THR:HG23	1:A:234:MET:H	1.83	0.42
1:B:44:LEU:HD11	1:B:54:ARG:HB2	2.01	0.42
1:C:89:PHE:O	1:C:213:ALA:HA	2.19	0.42
1:D:103:ASN:O	1:D:106:ASP:HB2	2.19	0.42
1:D:115:ARG:NH2	1:D:120:SER:O	2.52	0.42
1:E:44:LEU:HD12	1:E:52:SER:HB2	2.00	0.42
1:E:170:ASP:OD1	1:E:170:ASP:N	2.52	0.42
1:E:205:MET:C	1:E:209:GLN:HE21	2.23	0.42
1:A:156:THR:HG21	1:A:196:GLU:HG3	2.01	0.42
1:A:215:MET:HG2	2:A:305:HOH:O	2.17	0.42
1:D:161:THR:OG1	1:D:165:GLY:N	2.40	0.42
1:E:67:THR:O	1:E:73:SER:HB2	2.19	0.42
1:F:114:VAL:HG11	1:F:187:TRP:CH2	2.55	0.42
1:A:6:VAL:HG22	1:A:84:LEU:HD21	2.02	0.42
1:B:71:GLY:HA2	1:B:74:THR:HB	2.01	0.42
1:D:113:ALA:HB3	1:D:130:ALA:HB3	2.01	0.42
1:E:252:LEU:HA	1:E:252:LEU:HD23	1.80	0.42
1:B:39:ASP:O	1:B:56:GLU:N	2.39	0.42
1:B:106:ASP:O	1:B:219:VAL:N	2.48	0.42
1:D:224:THR:O	2:D:309:HOH:O	2.22	0.42
1:E:54:ARG:HG3	1:E:63:ILE:HD13	2.02	0.42
1:B:9:LEU:O	1:B:47:HIS:ND1	2.53	0.42
1:D:128:PHE:HE2	1:D:207:ALA:HB3	1.83	0.42
1:F:30:ARG:HG2	1:F:34:ILE:HD11	2.02	0.42
1:F:105:GLY:HA2	1:F:237:THR:OG1	2.20	0.42
1:F:196:GLU:CD	1:F:198:GLU:H	2.28	0.42
1:A:160:ASP:HB3	1:B:119:ALA:HA	2.01	0.42
1:C:22:ALA:HA	1:C:63:ILE:O	2.20	0.42
1:E:74:THR:O	1:E:78:VAL:HG23	2.18	0.42
1:E:75:SER:HA	1:E:205:MET:SD	2.60	0.42
1:F:159:SER:OG	1:F:165:GLY:HA3	2.19	0.42
1:A:28:PRO:HA	1:A:31:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:GLY:HA3	1:F:118:GLY:HA3	2.00	0.42
1:F:242:VAL:O	1:F:245:VAL:HG12	2.18	0.42
1:C:166:GLN:HA	1:C:195:TYR:CE1	2.54	0.42
1:C:98:ILE:HB	1:C:184:MET:HE1	2.01	0.42
1:F:5:ASP:OD1	1:F:12:THR:HG22	2.20	0.42
1:B:117:ASP:HA	1:B:160:ASP:HB2	2.02	0.41
1:C:98:ILE:HG22	1:C:223:ARG:HD3	2.02	0.41
1:B:161:THR:O	1:B:166:GLN:HG3	2.19	0.41
1:C:43:HIS:HE2	1:C:46:SER:HG	1.66	0.41
1:C:49:GLU:CG	1:D:49:GLU:HB2	2.43	0.41
1:C:92:ILE:HD13	1:C:93:GLY:N	2.34	0.41
1:C:143:ALA:HB1	1:C:247:GLU:HB3	2.02	0.41
1:E:115:ARG:HD2	1:E:130:ALA:HB2	2.02	0.41
1:F:185:GLU:HA	1:F:188:GLN:OE1	2.20	0.41
1:A:8:HIS:NE2	1:A:76:ILE:HD13	2.35	0.41
1:B:31:VAL:HG13	1:B:64:VAL:HG12	2.02	0.41
1:D:50:PHE:CE1	1:D:77:ALA:HB2	2.54	0.41
1:D:99:GLN:OE1	1:D:100:PRO:HD2	2.20	0.41
1:D:116:LEU:HD21	1:D:187:TRP:CZ2	2.55	0.41
1:A:44:LEU:HB2	1:A:52:SER:OG	2.20	0.41
1:C:71:GLY:N	1:C:72:PRO:HD2	2.36	0.41
1:D:84:LEU:HD23	1:D:84:LEU:HA	1.94	0.41
1:A:172:PHE:CD1	1:A:172:PHE:C	2.96	0.41
1:B:58:ASP:OD2	1:B:250:ARG:NH1	2.53	0.41
1:B:104:VAL:HG12	1:B:221:VAL:HA	2.02	0.41
1:C:9:LEU:HD23	1:C:80:GLU:HB2	2.02	0.41
1:E:5:ASP:HB2	1:E:12:THR:HA	2.02	0.41
1:C:123:PHE:CE1	1:D:164:PRO:HG3	2.55	0.41
1:E:123:PHE:CE2	1:E:205:MET:HE3	2.55	0.41
1:F:27:ASP:HA	1:F:28:PRO:HD3	1.95	0.41
1:F:75:SER:HA	1:F:205:MET:SD	2.61	0.41
1:A:88:THR:OG1	1:A:212:ARG:NE	2.52	0.41
1:A:110:THR:HA	1:A:154:GLY:O	2.21	0.41
1:A:165:GLY:HA2	1:A:180:PHE:CE1	2.56	0.41
1:D:233:THR:HG23	1:D:234:MET:N	2.36	0.41
1:E:16:LEU:HD22	1:E:63:ILE:CD1	2.51	0.41
1:E:104:VAL:HG11	1:E:229:PRO:HG3	2.03	0.41
1:F:175:ARG:HG2	1:F:176:VAL:N	2.34	0.41
1:D:183:SER:O	1:D:187:TRP:CD1	2.73	0.41
1:E:209:GLN:HG2	1:F:173:SER:CB	2.49	0.41
1:B:37:LEU:HD12	1:B:242:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLY:HA2	1:B:219:VAL:HG13	2.03	0.41
1:C:99:GLN:HB2	1:C:102:ILE:HD12	2.02	0.41
1:C:130:ALA:HB2	1:C:204:THR:OG1	2.20	0.41
1:D:53:TRP:N	1:D:64:VAL:O	2.47	0.41
1:D:108:LEU:HD13	1:D:193:MET:HB3	2.01	0.41
1:D:128:PHE:HD2	1:D:204:THR:HG23	1.85	0.41
1:E:15:ASP:O	1:E:54:ARG:NH1	2.54	0.41
1:E:35:ALA:O	1:E:41:PRO:HB3	2.21	0.41
1:E:47:HIS:O	1:E:48:ARG:HB2	2.21	0.41
1:F:117:ASP:HB2	1:F:160:ASP:OD1	2.20	0.41
1:F:128:PHE:HE1	1:F:207:ALA:HB3	1.86	0.41
1:F:178:ARG:HA	1:F:181:LYS:HB2	2.03	0.41
1:A:34:ILE:HB	1:A:64:VAL:HG11	2.03	0.41
1:A:41:PRO:HB2	1:A:53:TRP:HZ3	1.83	0.41
1:A:173:SER:C	1:A:175:ARG:N	2.77	0.41
1:B:143:ALA:O	1:B:147:VAL:HG23	2.21	0.41
1:C:8:HIS:HB3	1:C:50:PHE:CE2	2.56	0.41
1:D:94:THR:HB	1:D:220:ILE:CG2	2.51	0.41
1:D:125:PRO:C	1:D:127:GLU:H	2.28	0.41
1:D:167:GLU:HG3	1:D:176:VAL:HG11	2.03	0.41
1:F:30:ARG:O	1:F:34:ILE:N	2.50	0.41
1:A:99:GLN:HA	1:A:100:PRO:HD2	1.89	0.40
1:B:185:GLU:H	1:B:185:GLU:HG3	1.57	0.40
1:C:105:GLY:HA2	1:C:237:THR:CG2	2.51	0.40
1:D:57:LEU:HG	1:D:58:ASP:OD1	2.21	0.40
1:F:99:GLN:NE2	1:F:188:GLN:O	2.54	0.40
1:A:120:SER:C	1:A:122:HIS:N	2.80	0.40
1:C:177:VAL:O	1:C:180:PHE:N	2.54	0.40
1:D:93:GLY:O	1:D:217:ALA:HA	2.21	0.40
1:D:154:GLY:C	1:D:193:MET:HE2	2.47	0.40
1:D:169:TYR:C	1:D:171:THR:H	2.28	0.40
1:E:167:GLU:HB2	1:E:184:MET:HG2	2.03	0.40
1:A:40:ASN:N	1:A:41:PRO:HD3	2.37	0.40
1:A:196:GLU:OE2	1:A:199:SER:OG	2.28	0.40
1:B:8:HIS:HB2	1:B:80:GLU:OE2	2.22	0.40
1:C:158:SER:HB2	1:C:200:ALA:HB2	2.03	0.40
1:D:52:SER:HA	1:D:64:VAL:O	2.21	0.40
1:D:76:ILE:O	1:D:80:GLU:HB2	2.21	0.40
1:D:234:MET:HG2	1:D:238:GLU:HB2	2.03	0.40
1:A:48:ARG:NE	1:B:27:ASP:HB3	2.36	0.40
1:C:185:GLU:H	1:C:185:GLU:HG3	1.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:SER:C	1:A:122:HIS:H	2.29	0.40
1:B:97:ALA:HB2	1:B:219:VAL:HG11	2.03	0.40
1:C:165:GLY:CA	1:D:122:HIS:HD2	2.34	0.40
1:D:45:ALA:O	1:D:51:THR:HA	2.22	0.40
1:D:102:ILE:CG2	1:D:219:VAL:HG21	2.52	0.40
1:E:85:GLY:HA2	1:E:87:ARG:NH1	2.37	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	248/253 (98%)	228 (92%)	20 (8%)	0	100	100
1	B	248/253 (98%)	236 (95%)	11 (4%)	1 (0%)	30	28
1	C	248/253 (98%)	227 (92%)	17 (7%)	4 (2%)	7	3
1	D	248/253 (98%)	229 (92%)	18 (7%)	1 (0%)	30	28
1	E	248/253 (98%)	228 (92%)	18 (7%)	2 (1%)	16	12
1	F	248/253 (98%)	233 (94%)	15 (6%)	0	100	100
All	All	1488/1518 (98%)	1381 (93%)	99 (7%)	8 (0%)	24	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	MET
1	C	221	VAL
1	C	116	LEU
1	B	176	VAL
1	C	176	VAL
1	D	221	VAL

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Mol	Chain	Res	Type
1	E	229	PRO
1	E	176	VAL

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	201/203 (99%)	175 (87%)	26 (13%)	4	2
1	B	201/203 (99%)	170 (85%)	31 (15%)	2	1
1	C	201/203 (99%)	171 (85%)	30 (15%)	3	1
1	D	201/203 (99%)	170 (85%)	31 (15%)	2	1
1	E	201/203 (99%)	169 (84%)	32 (16%)	2	1
1	F	201/203 (99%)	181 (90%)	20 (10%)	7	4
All	All	1206/1218 (99%)	1036 (86%)	170 (14%)	3	1

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	6	VAL
1	A	12	THR
1	A	27	ASP
1	A	39	ASP
1	A	49	GLU
1	A	62	VAL
1	A	73	SER
1	A	75	SER
1	A	127	GLU
1	A	135	SER
1	A	160	ASP
1	A	171	THR
1	A	178	ARG
1	A	181	LYS
1	A	184	MET

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Mol	Chain	Res	Type
1	A	185	GLU
1	A	186	GLU
1	A	202	LEU
1	A	220	ILE
1	A	227	GLU
1	A	235	LYS
1	A	238	GLU
1	A	247	GLU
1	A	250	ARG
1	A	252	LEU
1	B	12	THR
1	B	17	GLN
1	B	42	VAL
1	B	49	GLU
1	B	56	GLU
1	B	62	VAL
1	B	92	ILE
1	B	95	THR
1	B	110	THR
1	B	145	LYS
1	B	151	THR
1	B	160	ASP
1	B	170	ASP
1	B	171	THR
1	B	175	ARG
1	B	177	VAL
1	B	183	SER
1	B	185	GLU
1	B	188	GLN
1	B	195	TYR
1	B	196	GLU
1	B	204	THR
1	B	209	GLN
1	B	227	GLU
1	B	228	ILE
1	B	230	ASN
1	B	231	GLU
1	B	233	THR
1	B	234	MET
1	B	244	ILE
1	B	245	VAL
1	C	9	LEU

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Mol	Chain	Res	Type
1	C	24	VAL
1	C	37	LEU
1	C	52	SER
1	C	57	LEU
1	C	60	LYS
1	C	69	ILE
1	C	72	PRO
1	C	75	SER
1	C	76	ILE
1	C	92	ILE
1	C	98	ILE
1	C	117	ASP
1	C	135	SER
1	C	146	SER
1	C	167	GLU
1	C	168	ARG
1	C	169	TYR
1	C	172	PHE
1	C	176	VAL
1	C	185	GLU
1	C	188	GLN
1	C	201	THR
1	C	226	GLN
1	C	230	ASN
1	C	231	GLU
1	C	233	THR
1	C	234	MET
1	C	238	GLU
1	C	242	VAL
1	D	6	VAL
1	D	9	LEU
1	D	14	ASN
1	D	17	GLN
1	D	20	THR
1	D	27	ASP
1	D	37	LEU
1	D	48	ARG
1	D	52	SER
1	D	54	ARG
1	D	58	ASP
1	D	80	GLU
1	D	135	SER

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Mol	Chain	Res	Type
1	D	138	THR
1	D	147	VAL
1	D	151	THR
1	D	170	ASP
1	D	172	PHE
1	D	176	VAL
1	D	177	VAL
1	D	189	SER
1	D	195	TYR
1	D	196	GLU
1	D	206	CYS
1	D	208	SER
1	D	224	THR
1	D	228	ILE
1	D	230	ASN
1	D	235	LYS
1	D	240	HIS
1	D	250	ARG
1	E	6	VAL
1	E	11	LEU
1	E	12	THR
1	E	13	LYS
1	E	21	LEU
1	E	23	ILE
1	E	37	LEU
1	E	48	ARG
1	E	52	SER
1	E	56	GLU
1	E	64	VAL
1	E	73	SER
1	E	92	ILE
1	E	106	ASP
1	E	135	SER
1	E	153	ILE
1	E	158	SER
1	E	167	GLU
1	E	170	ASP
1	E	172	PHE
1	E	175	ARG
1	E	185	GLU
1	E	188	GLN
1	E	193	MET

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Mol	Chain	Res	Type
1	E	196	GLU
1	E	226	GLN
1	E	233	THR
1	E	234	MET
1	E	235	LYS
1	E	237	THR
1	E	240	HIS
1	E	247	GLU
1	F	4	SER
1	F	5	ASP
1	F	11	LEU
1	F	16	LEU
1	F	24	VAL
1	F	62	VAL
1	F	138	THR
1	F	147	VAL
1	F	156	THR
1	F	158	SER
1	F	170	ASP
1	F	172	PHE
1	F	181	LYS
1	F	185	GLU
1	F	196	GLU
1	F	201	THR
1	F	221	VAL
1	F	228	ILE
1	F	242	VAL
1	F	250	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	152	HIS
1	A	209	GLN
1	B	99	GLN
1	B	225	GLN
1	D	8	HIS
1	D	251	HIS
1	F	152	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	250/253 (98%)	-1.00	0 100 100	17, 31, 50, 61	0
1	B	250/253 (98%)	-1.05	0 100 100	16, 30, 44, 55	0
1	C	250/253 (98%)	-1.05	0 100 100	18, 30, 46, 53	0
1	D	250/253 (98%)	-1.06	0 100 100	16, 31, 46, 58	0
1	E	250/253 (98%)	-1.00	0 100 100	20, 32, 53, 66	0
1	F	250/253 (98%)	-1.03	0 100 100	19, 34, 50, 59	0
All	All	1500/1518 (98%)	-1.03	0 100 100	16, 32, 50, 66	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.