Full wwPDB X-ray Structure Validation Report (i)

May 28, 2020 – 08:55 pm BST

PDB ID	:	1VZ0
Title	:	Chromosome segregation protein Spo0J from Thermus thermophilus
Authors	:	Leonard, T.A.; Butler, P.J.G.; Lowe, J.
Deposited on	:	2004-05-12
Resolution	:	2.30 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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.
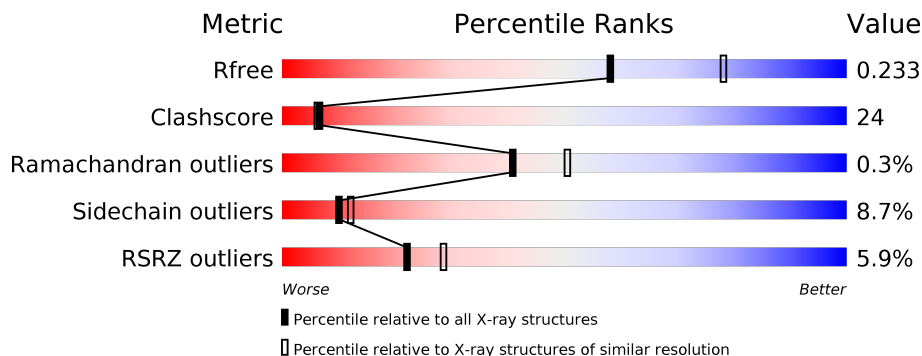
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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 <=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	230	3% / 56% 19% 7% 19%
1	B	230	6% / 48% 33% • 16%
1	C	230	3% / 53% 27% • 17%
1	D	230	5% / 59% 23% • 16%
1	E	230	7% / 57% 22% 5% 17%
1	F	230	2% / 54% 26% • 18%

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Mol	Chain	Length	Quality of chain
1	G	230	8%　50%　27%　·　19%
1	H	230	4%　56%　23%　·　18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12878 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 Chromosome-partitioning protein Spo0J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	0	1
			1459	911	272	273	3			
1	B	193	Total	C	N	O	S	0	0	1
			1511	943	284	281	3			
1	C	190	Total	C	N	O	S	0	0	1
			1487	928	278	278	3			
1	D	193	Total	C	N	O	S	0	0	1
			1511	943	284	281	3			
1	E	192	Total	C	N	O	S	0	0	1
			1506	940	283	280	3			
1	F	189	Total	C	N	O	S	0	0	1
			1478	923	277	275	3			
1	G	187	Total	C	N	O	S	0	0	1
			1459	911	272	273	3			
1	H	188	Total	C	N	O	S	0	0	1
			1467	917	273	274	3			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLY	-	expression tag	UNP Q72H91
A	224	SER	-	expression tag	UNP Q72H91
A	225	HIS	-	expression tag	UNP Q72H91
A	226	HIS	-	expression tag	UNP Q72H91
A	227	HIS	-	expression tag	UNP Q72H91
A	228	HIS	-	expression tag	UNP Q72H91
A	229	HIS	-	expression tag	UNP Q72H91
A	230	HIS	-	expression tag	UNP Q72H91
B	223	GLY	-	expression tag	UNP Q72H91
B	224	SER	-	expression tag	UNP Q72H91
B	225	HIS	-	expression tag	UNP Q72H91
B	226	HIS	-	expression tag	UNP Q72H91
B	227	HIS	-	expression tag	UNP Q72H91

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Chain	Residue	Modelled	Actual	Comment	Reference
B	228	HIS	-	expression tag	UNP Q72H91
B	229	HIS	-	expression tag	UNP Q72H91
B	230	HIS	-	expression tag	UNP Q72H91
C	223	GLY	-	expression tag	UNP Q72H91
C	224	SER	-	expression tag	UNP Q72H91
C	225	HIS	-	expression tag	UNP Q72H91
C	226	HIS	-	expression tag	UNP Q72H91
C	227	HIS	-	expression tag	UNP Q72H91
C	228	HIS	-	expression tag	UNP Q72H91
C	229	HIS	-	expression tag	UNP Q72H91
C	230	HIS	-	expression tag	UNP Q72H91
D	223	GLY	-	expression tag	UNP Q72H91
D	224	SER	-	expression tag	UNP Q72H91
D	225	HIS	-	expression tag	UNP Q72H91
D	226	HIS	-	expression tag	UNP Q72H91
D	227	HIS	-	expression tag	UNP Q72H91
D	228	HIS	-	expression tag	UNP Q72H91
D	229	HIS	-	expression tag	UNP Q72H91
D	230	HIS	-	expression tag	UNP Q72H91
E	223	GLY	-	expression tag	UNP Q72H91
E	224	SER	-	expression tag	UNP Q72H91
E	225	HIS	-	expression tag	UNP Q72H91
E	226	HIS	-	expression tag	UNP Q72H91
E	227	HIS	-	expression tag	UNP Q72H91
E	228	HIS	-	expression tag	UNP Q72H91
E	229	HIS	-	expression tag	UNP Q72H91
E	230	HIS	-	expression tag	UNP Q72H91
F	223	GLY	-	expression tag	UNP Q72H91
F	224	SER	-	expression tag	UNP Q72H91
F	225	HIS	-	expression tag	UNP Q72H91
F	226	HIS	-	expression tag	UNP Q72H91
F	227	HIS	-	expression tag	UNP Q72H91
F	228	HIS	-	expression tag	UNP Q72H91
F	229	HIS	-	expression tag	UNP Q72H91
F	230	HIS	-	expression tag	UNP Q72H91
G	223	GLY	-	expression tag	UNP Q72H91
G	224	SER	-	expression tag	UNP Q72H91
G	225	HIS	-	expression tag	UNP Q72H91
G	226	HIS	-	expression tag	UNP Q72H91
G	227	HIS	-	expression tag	UNP Q72H91
G	228	HIS	-	expression tag	UNP Q72H91
G	229	HIS	-	expression tag	UNP Q72H91

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Chain	Residue	Modelled	Actual	Comment	Reference
G	230	HIS	-	expression tag	UNP Q72H91
H	223	GLY	-	expression tag	UNP Q72H91
H	224	SER	-	expression tag	UNP Q72H91
H	225	HIS	-	expression tag	UNP Q72H91
H	226	HIS	-	expression tag	UNP Q72H91
H	227	HIS	-	expression tag	UNP Q72H91
H	228	HIS	-	expression tag	UNP Q72H91
H	229	HIS	-	expression tag	UNP Q72H91
H	230	HIS	-	expression tag	UNP Q72H91

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Co 1	0	0
2	D	2	Total 2	Co 2	0	0
2	E	2	Total 2	Co 2	0	0
2	H	1	Total 1	Co 1	0	0
2	B	2	Total 2	Co 2	0	0
2	C	2	Total 2	Co 2	0	0
2	A	3	Total 3	Co 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total 140	O 140	0	0

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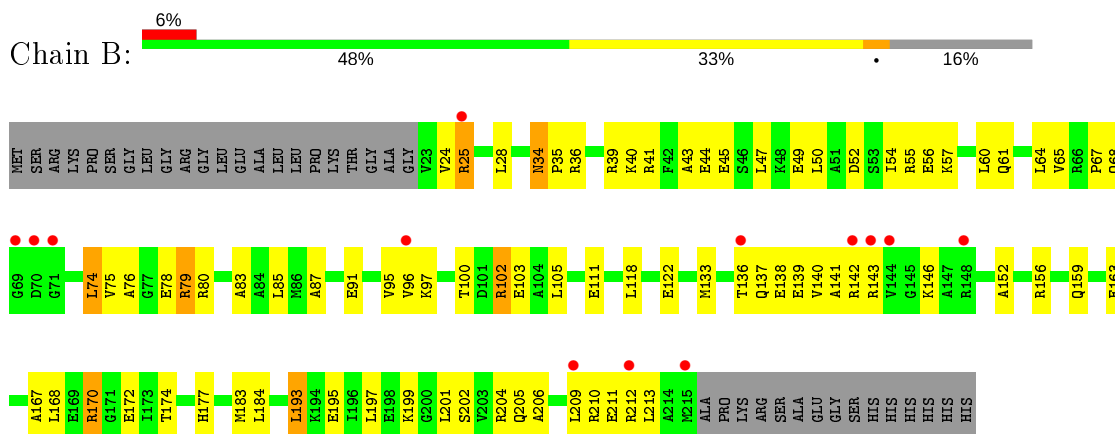| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	130	Total 130	O 130	0	0
4	C	114	Total 114	O 114	0	0
4	D	126	Total 126	O 126	0	0
4	E	110	Total 110	O 110	0	0
4	F	117	Total 117	O 117	0	0
4	G	122	Total 122	O 122	0	0
4	H	126	Total 126	O 126	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Chromosome-partitioning protein Spo0J
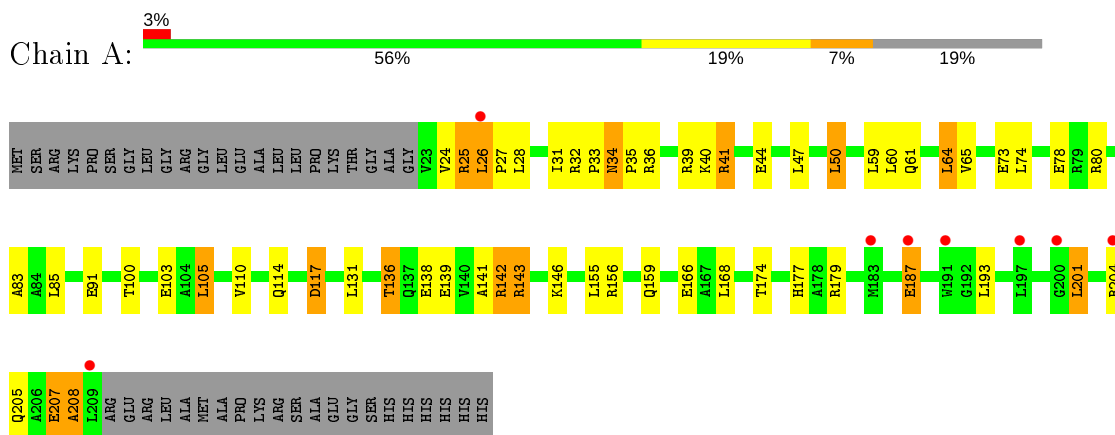
Chain A:

- Molecule 1: Chromosome-partitioning protein Spo0J

Chain B:

- Molecule 1: Chromosome-partitioning protein Spo0J

Chain C:

● Molecule 1: Chromosome-partitioning protein Spo0J

Chain D:

● Molecule 1: Chromosome-partitioning protein Spo0J

Chain E:

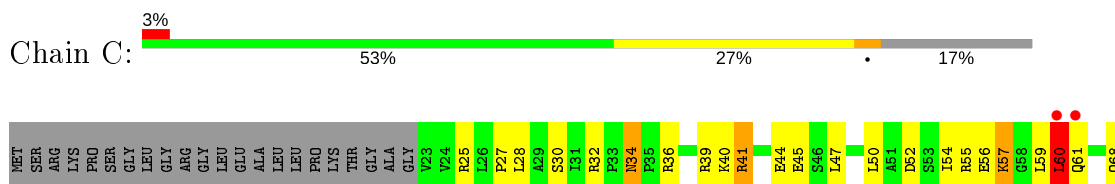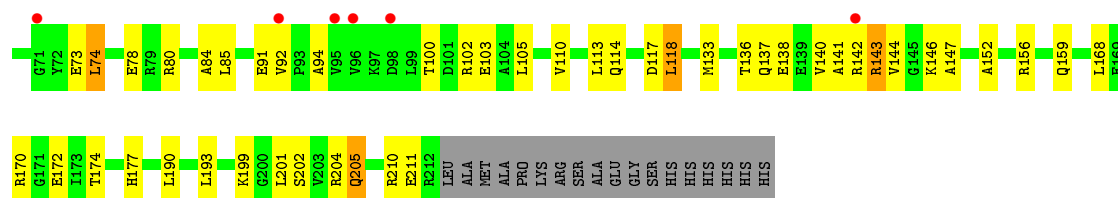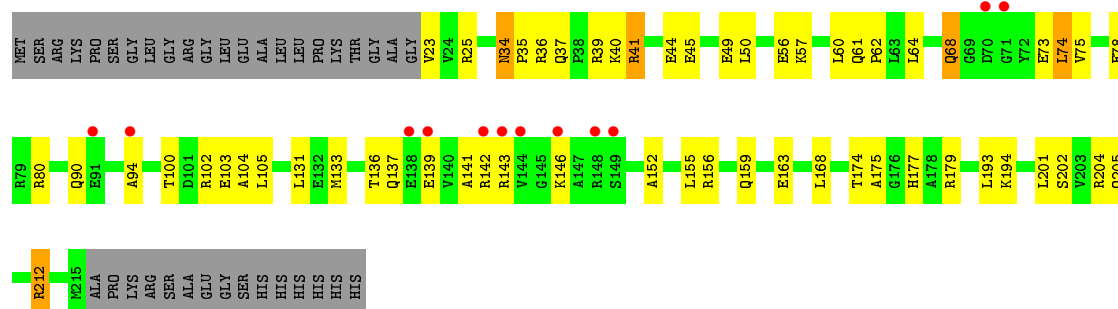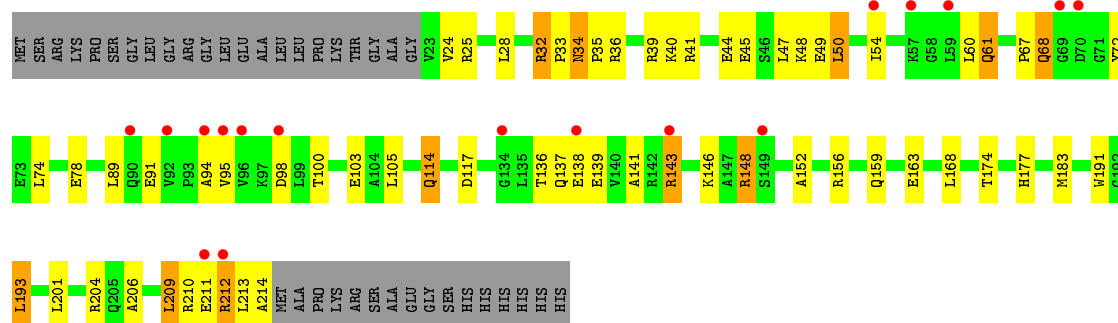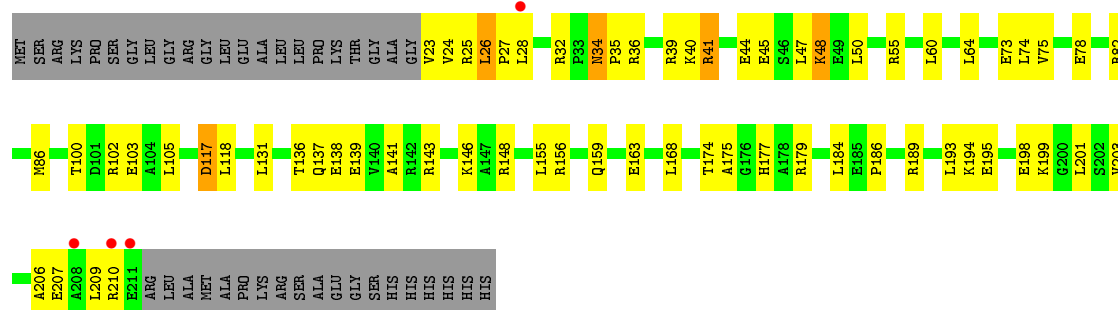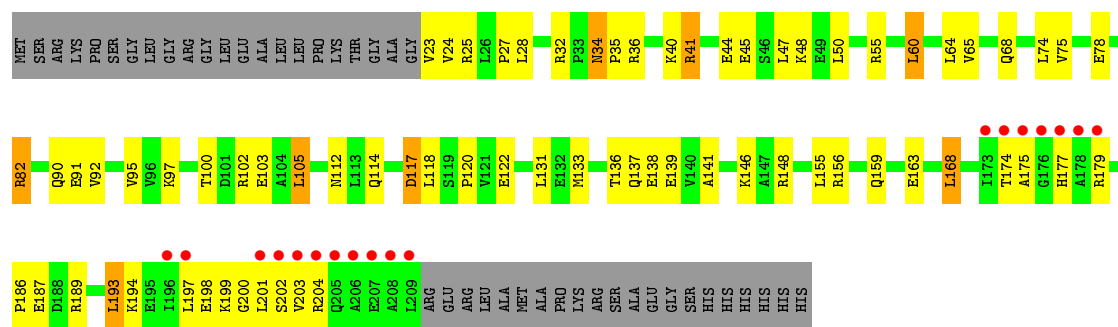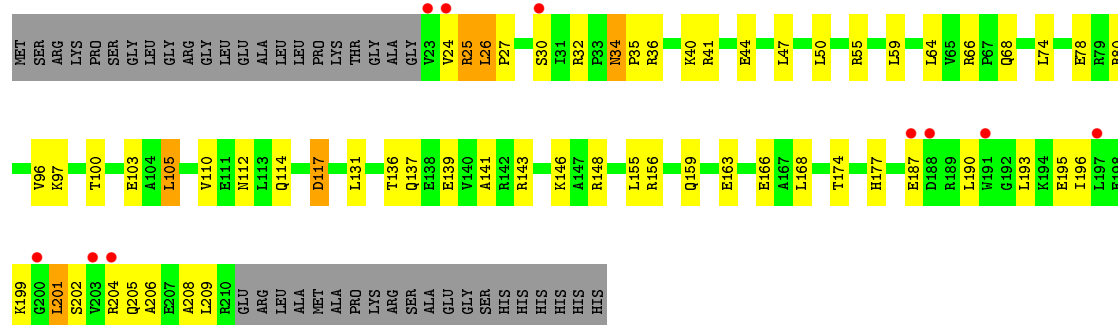● Molecule 1: Chromosome-partitioning protein Spo0J

Chain F:

● Molecule 1: Chromosome-partitioning protein Spo0J

Chain G:

• Molecule 1: Chromosome-partitioning protein Spo0J

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	182.24Å　　295.15Å　　73.49Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	38.72　–　2.30 155.06　–　2.29	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.72-2.30) 98.2 (155.06-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.47 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235　,　0.278 0.231　,　0.233	Depositor DCC
R_{free} test set	4470 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.5	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12878	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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 25.31 % 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 3.2475e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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, CO

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	0.36	0/1476	0.62	0/1993
1	B	0.33	0/1528	0.63	1/2062 (0.0%)
1	C	0.34	0/1504	0.62	0/2030
1	D	0.33	0/1528	0.58	0/2062
1	E	0.33	0/1523	0.62	0/2055
1	F	0.35	0/1495	0.60	0/2018
1	G	0.36	0/1476	0.64	1/1993 (0.1%)
1	H	0.36	0/1484	0.61	0/2004
All	All	0.34	0/12014	0.61	2/16217 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	79	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	G	82	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1459	0	1517	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1511	0	1576	94	0
1	C	1487	0	1547	90	0
1	D	1511	0	1576	71	0
1	E	1506	0	1571	81	0
1	F	1478	0	1541	69	0
1	G	1459	0	1517	91	0
1	H	1467	0	1528	80	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	140	0	0	7	0
4	B	130	0	0	17	0
4	C	114	0	0	11	0
4	D	126	0	0	8	0
4	E	110	0	0	11	0
4	F	117	0	0	8	0
4	G	122	0	0	13	0
4	H	126	0	0	3	0
All	All	12878	0	12373	573	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 24.

All (573) 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:C:25:ARG:HH21	1:C:25:ARG:HB3	1.12	1.11
1:G:64:LEU:HG	1:G:97:LYS:HZ1	1.14	1.06
1:A:142:ARG:HA	1:A:142:ARG:HE	1.20	1.01
1:D:94:ALA:HB3	1:H:26:LEU:HD21	1.42	1.01
1:B:202:SER:H	1:B:205:GLN:HE21	1.03	0.98
1:D:202:SER:H	1:D:205:GLN:HE21	1.09	0.94
1:G:64:LEU:HD22	1:G:75:VAL:HB	1.51	0.91
1:G:174:THR:H	1:G:177:HIS:HD2	1.14	0.90
1:B:118:LEU:HA	4:B:2068:HOH:O	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:LEU:HG	1:G:97:LYS:NZ	1.87	0.88
1:H:174:THR:H	1:H:177:HIS:HD2	1.22	0.88
1:H:25:ARG:HH21	1:H:25:ARG:HB3	1.38	0.88
1:C:25:ARG:NH2	1:C:25:ARG:HB3	1.90	0.87
1:E:213:LEU:HD23	1:E:214:ALA:N	1.90	0.86
1:E:136:THR:HB	1:E:139:GLU:HG2	1.58	0.86
1:E:174:THR:H	1:E:177:HIS:HD2	1.22	0.86
1:A:117:ASP:HB3	1:C:39:ARG:HH22	1.42	0.84
1:F:174:THR:H	1:F:177:HIS:HD2	1.21	0.83
1:B:174:THR:H	1:B:177:HIS:HD2	1.22	0.83
1:B:78:GLU:HG2	4:B:2043:HOH:O	1.77	0.83
1:C:60:LEU:H	1:C:60:LEU:HD23	1.44	0.83
1:A:142:ARG:NE	1:A:142:ARG:HA	1.92	0.82
1:D:39:ARG:HH22	1:H:117:ASP:HB3	1.42	0.82
1:G:193:LEU:HB3	4:G:2119:HOH:O	1.80	0.81
1:A:174:THR:H	1:A:177:HIS:HD2	1.23	0.81
1:C:25:ARG:CB	1:C:25:ARG:HH21	1.93	0.81
1:A:136:THR:HG22	1:A:139:GLU:H	1.44	0.80
1:H:196:ILE:HA	1:H:201:LEU:HB2	1.60	0.80
1:E:143:ARG:HD2	1:E:143:ARG:H	1.45	0.80
1:F:64:LEU:HD12	1:F:75:VAL:HB	1.64	0.80
1:F:24:VAL:HG12	1:F:25:ARG:H	1.46	0.79
1:G:156:ARG:O	1:G:159:GLN:HG2	1.81	0.79
1:B:25:ARG:HH12	1:G:91:GLU:HB3	1.47	0.79
1:F:156:ARG:O	1:F:159:GLN:HG2	1.83	0.79
1:C:174:THR:H	1:C:177:HIS:HD2	1.30	0.79
1:H:208:ALA:O	1:H:209:LEU:HD12	1.82	0.79
1:A:201:LEU:H	1:A:201:LEU:HD23	1.48	0.79
1:B:202:SER:H	1:B:205:GLN:NE2	1.78	0.79
1:B:39:ARG:HH22	1:G:117:ASP:HB3	1.48	0.78
1:D:202:SER:H	1:D:205:GLN:NE2	1.80	0.78
1:B:85:LEU:HD21	1:G:28:LEU:HD21	1.66	0.77
1:D:34:ASN:ND2	1:D:36:ARG:HH21	1.82	0.77
1:D:68:GLN:HG2	1:H:32:ARG:HH21	1.47	0.76
1:E:32:ARG:HB3	1:E:32:ARG:HH11	1.51	0.76
1:E:39:ARG:HH22	1:F:117:ASP:HB3	1.49	0.75
1:H:156:ARG:O	1:H:159:GLN:HG2	1.85	0.75
1:G:64:LEU:CG	1:G:97:LYS:HZ1	1.97	0.75
1:G:174:THR:H	1:G:177:HIS:CD2	2.02	0.75
1:H:34:ASN:ND2	1:H:36:ARG:H	1.84	0.75
1:D:174:THR:H	1:D:177:HIS:HD2	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:VAL:O	1:A:114:GLN:HG2	1.87	0.74
1:B:85:LEU:CD2	1:G:28:LEU:HD21	2.17	0.74
1:B:202:SER:N	1:B:205:GLN:HE21	1.84	0.74
1:A:28:LEU:HD21	1:C:85:LEU:CD2	2.18	0.74
1:D:34:ASN:HD21	1:D:36:ARG:HH21	1.33	0.73
1:D:156:ARG:O	1:D:159:GLN:HG2	1.89	0.73
1:G:24:VAL:HG12	1:G:25:ARG:N	2.02	0.73
1:B:201:LEU:HA	1:B:205:GLN:NE2	2.04	0.72
1:G:34:ASN:ND2	1:G:36:ARG:H	1.86	0.72
1:H:34:ASN:ND2	1:H:36:ARG:HH21	1.87	0.72
1:A:34:ASN:ND2	1:A:36:ARG:H	1.87	0.72
1:F:34:ASN:ND2	1:F:36:ARG:HH21	1.88	0.72
1:B:136:THR:HB	1:B:139:GLU:OE2	1.89	0.71
1:B:156:ARG:O	1:B:159:GLN:HG2	1.89	0.71
1:B:193:LEU:HD13	1:G:60:LEU:HD11	1.71	0.71
1:A:34:ASN:ND2	1:A:36:ARG:HH21	1.88	0.71
1:F:64:LEU:CD1	1:F:75:VAL:HB	2.20	0.71
1:E:211:GLU:HG3	4:E:2106:HOH:O	1.90	0.71
1:F:206:ALA:O	1:F:209:LEU:HD23	1.89	0.71
1:C:156:ARG:O	1:C:159:GLN:HG2	1.90	0.71
1:E:143:ARG:H	1:E:143:ARG:CD	2.02	0.71
1:B:34:ASN:ND2	1:B:36:ARG:H	1.87	0.71
1:H:174:THR:H	1:H:177:HIS:CD2	2.09	0.71
1:B:64:LEU:HD21	1:B:97:LYS:HD2	1.72	0.70
1:A:28:LEU:HD21	1:C:85:LEU:HD21	1.73	0.70
1:F:24:VAL:HG12	1:F:25:ARG:N	2.05	0.70
1:C:210:ARG:NH1	1:F:131:LEU:O	2.21	0.70
1:A:156:ARG:O	1:A:159:GLN:HG2	1.91	0.70
1:A:166:GLU:HG2	4:A:2123:HOH:O	1.91	0.70
1:F:194:LYS:O	1:F:198:GLU:HG2	1.92	0.70
1:B:25:ARG:HB3	1:B:25:ARG:CZ	2.21	0.70
1:C:199:LYS:HB2	1:C:201:LEU:HD13	1.73	0.70
1:G:24:VAL:HG12	1:G:25:ARG:H	1.55	0.70
1:E:68:GLN:HE21	1:E:68:GLN:HA	1.56	0.69
1:B:25:ARG:CZ	4:B:2001:HOH:O	2.39	0.69
1:B:78:GLU:OE2	4:B:2042:HOH:O	2.09	0.69
1:B:39:ARG:NH1	1:G:118:LEU:HD23	2.07	0.69
1:E:174:THR:H	1:E:177:HIS:CD2	2.08	0.69
1:G:28:LEU:HD23	1:G:28:LEU:O	1.93	0.69
1:A:201:LEU:HB2	1:A:205:GLN:HB2	1.73	0.69
1:E:34:ASN:ND2	1:E:36:ARG:H	1.89	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD22	1:A:80:ARG:HG2	1.75	0.69
4:A:2131:HOH:O	1:C:61:GLN:HG3	1.93	0.69
1:E:34:ASN:ND2	1:E:36:ARG:HH21	1.90	0.69
1:A:60:LEU:HD13	1:A:61:GLN:HG3	1.74	0.68
1:C:60:LEU:HG	1:C:61:GLN:H	1.59	0.68
1:C:102:ARG:HH12	1:C:133:MET:HB3	1.58	0.68
1:F:174:THR:H	1:F:177:HIS:CD2	2.10	0.68
1:C:102:ARG:NH1	1:C:133:MET:O	2.27	0.67
1:C:141:ALA:HB1	1:C:146:LYS:O	1.93	0.67
1:B:52:ASP:HA	1:B:55:ARG:NH2	2.09	0.67
1:E:91:GLU:HG2	1:F:27:PRO:HA	1.76	0.67
1:H:202:SER:H	1:H:205:GLN:NE2	1.93	0.67
1:F:136:THR:HG23	1:F:139:GLU:H	1.60	0.67
1:B:34:ASN:ND2	1:B:36:ARG:HH21	1.93	0.67
1:H:24:VAL:HG12	1:H:25:ARG:N	2.10	0.66
4:D:2085:HOH:O	1:H:114:GLN:HB3	1.95	0.66
1:B:174:THR:H	1:B:177:HIS:CD2	2.09	0.66
1:H:34:ASN:HD21	1:H:36:ARG:HH21	1.44	0.66
1:A:34:ASN:HD21	1:A:36:ARG:HH21	1.44	0.66
1:A:142:ARG:NH2	1:H:55:ARG:HE	1.94	0.66
1:B:25:ARG:HH11	1:G:92:VAL:C	1.98	0.66
1:F:138:GLU:HG3	4:G:2031:HOH:O	1.96	0.66
1:A:32:ARG:HB2	1:A:33:PRO:HD2	1.77	0.66
1:D:57:LYS:HZ3	1:H:190:LEU:HD11	1.61	0.66
1:E:25:ARG:HH21	1:E:25:ARG:HG3	1.61	0.66
1:D:78:GLU:OE1	1:H:34:ASN:HB3	1.96	0.66
1:D:73:GLU:OE2	1:H:36:ARG:NH1	2.28	0.65
1:D:34:ASN:ND2	1:D:36:ARG:NH2	2.43	0.65
1:E:213:LEU:HB3	4:E:2105:HOH:O	1.96	0.65
1:E:50:LEU:O	1:E:54:ILE:HG13	1.96	0.65
1:H:68:GLN:HA	1:H:68:GLN:HE21	1.62	0.65
1:C:34:ASN:ND2	1:C:36:ARG:HH21	1.95	0.65
1:B:60:LEU:HD11	4:G:2119:HOH:O	1.96	0.65
1:F:34:ASN:HD21	1:F:36:ARG:HH21	1.42	0.65
1:B:25:ARG:HB3	1:B:25:ARG:NH2	2.11	0.65
1:C:34:ASN:HD21	1:C:36:ARG:HH21	1.44	0.64
4:F:2071:HOH:O	1:G:90:GLN:HG3	1.96	0.64
1:F:40:LYS:O	1:F:44:GLU:HG3	1.96	0.64
1:C:32:ARG:NE	4:C:2004:HOH:O	2.31	0.64
1:E:68:GLN:HG3	1:F:32:ARG:NH1	2.13	0.64
1:H:40:LYS:O	1:H:44:GLU:HG3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:HH21	1:A:204:ARG:HG3	1.63	0.64
1:D:179:ARG:NH1	4:D:2090:HOH:O	2.30	0.64
1:A:91:GLU:OE2	1:C:25:ARG:NE	2.31	0.64
1:G:175:ALA:HB2	4:G:2112:HOH:O	1.97	0.64
1:A:26:LEU:HD13	1:A:31:ILE:HD11	1.79	0.63
1:A:34:ASN:ND2	1:A:36:ARG:NH2	2.46	0.63
1:G:194:LYS:O	1:G:198:GLU:HB2	1.97	0.63
1:B:25:ARG:NH1	1:G:91:GLU:HB3	2.14	0.63
1:B:78:GLU:OE1	1:G:34:ASN:HB3	1.98	0.63
1:C:159:GLN:HB3	4:C:2032:HOH:O	1.99	0.63
1:G:198:GLU:HA	1:G:201:LEU:CD2	2.28	0.63
1:A:136:THR:CG2	1:A:138:GLU:HB3	2.29	0.62
1:D:139:GLU:O	1:D:143:ARG:HG2	1.99	0.62
1:G:137:GLN:HE21	1:G:148:ARG:HE	1.47	0.62
1:B:91:GLU:HG2	1:G:27:PRO:HA	1.80	0.62
1:C:202:SER:H	1:C:205:GLN:CG	2.12	0.62
1:D:23:VAL:N	4:D:2001:HOH:O	2.32	0.62
1:A:174:THR:H	1:A:177:HIS:CD2	2.12	0.62
1:A:26:LEU:CD1	1:A:31:ILE:HD11	2.29	0.62
1:D:174:THR:H	1:D:177:HIS:CD2	2.17	0.62
1:H:136:THR:HG23	1:H:139:GLU:H	1.64	0.62
1:D:68:GLN:CG	1:H:32:ARG:HH21	2.13	0.62
1:C:174:THR:H	1:C:177:HIS:CD2	2.15	0.62
1:B:25:ARG:HH12	1:G:91:GLU:CB	2.13	0.62
1:H:136:THR:HG22	1:H:139:GLU:CG	2.29	0.62
1:H:202:SER:HB2	1:H:205:GLN:HG3	1.82	0.62
1:B:141:ALA:HB1	1:B:146:LYS:O	1.99	0.62
1:F:34:ASN:ND2	1:F:36:ARG:H	1.98	0.62
1:G:40:LYS:O	1:G:44:GLU:HG3	2.00	0.62
1:D:68:GLN:HE21	1:D:68:GLN:HA	1.63	0.62
1:G:48:LYS:HE2	4:G:2028:HOH:O	1.99	0.62
1:B:211:GLU:N	4:B:2122:HOH:O	2.32	0.61
1:E:183:MET:HB3	1:E:210:ARG:HD2	1.82	0.61
1:F:34:ASN:ND2	1:F:36:ARG:NH2	2.48	0.61
1:H:110:VAL:O	1:H:114:GLN:HG3	1.99	0.61
1:H:201:LEU:HD13	1:H:205:GLN:HE21	1.65	0.61
1:A:40:LYS:O	1:A:44:GLU:HG3	2.00	0.61
1:E:136:THR:H	1:E:139:GLU:CG	2.12	0.61
1:E:212:ARG:O	1:E:212:ARG:HG2	2.01	0.61
1:D:136:THR:HG22	1:D:139:GLU:HG3	1.82	0.61
1:G:136:THR:HG22	1:G:138:GLU:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:THR:HG22	1:H:139:GLU:HG3	1.82	0.61
1:C:147:ALA:HB1	4:C:2067:HOH:O	1.99	0.61
1:H:25:ARG:NH2	1:H:25:ARG:HB3	2.13	0.61
4:C:2074:HOH:O	1:F:136:THR:HG21	2.00	0.61
1:H:34:ASN:ND2	1:H:36:ARG:NH2	2.49	0.61
1:E:34:ASN:ND2	1:E:36:ARG:NH2	2.49	0.60
1:B:52:ASP:HA	1:B:55:ARG:HH22	1.65	0.60
1:D:202:SER:N	1:D:205:GLN:HE21	1.92	0.60
1:H:100:THR:OG1	1:H:103:GLU:HG3	2.01	0.60
1:D:136:THR:HG23	1:D:139:GLU:H	1.66	0.60
1:D:68:GLN:HG2	1:H:32:ARG:NH2	2.17	0.60
1:B:183:MET:HE3	4:B:2121:HOH:O	2.01	0.60
1:E:34:ASN:HD21	1:E:36:ARG:HH21	1.49	0.60
1:H:202:SER:HB2	1:H:205:GLN:CG	2.32	0.60
1:H:206:ALA:O	1:H:209:LEU:HD13	2.00	0.60
1:D:64:LEU:HD22	1:D:75:VAL:HB	1.83	0.60
1:B:212:ARG:HB3	4:B:2123:HOH:O	2.01	0.59
1:B:64:LEU:HB3	1:B:76:ALA:HB3	1.83	0.59
1:F:201:LEU:HA	4:F:2116:HOH:O	2.01	0.59
1:C:202:SER:OG	1:C:205:GLN:HG2	2.02	0.59
1:A:28:LEU:HD23	1:A:28:LEU:C	2.23	0.59
1:B:100:THR:OG1	1:B:103:GLU:HG3	2.03	0.59
1:E:114:GLN:HG3	4:E:2054:HOH:O	2.00	0.59
4:B:2094:HOH:O	1:G:114:GLN:HB3	2.02	0.59
1:D:137:GLN:HE22	1:D:152:ALA:HB2	1.67	0.58
1:H:141:ALA:HB1	1:H:146:LYS:O	2.03	0.58
1:E:100:THR:OG1	1:E:103:GLU:HG3	2.03	0.58
1:E:211:GLU:C	1:E:213:LEU:H	2.05	0.58
1:G:198:GLU:HA	1:G:201:LEU:HD21	1.84	0.58
1:G:28:LEU:C	1:G:28:LEU:HD23	2.24	0.58
1:E:156:ARG:O	1:E:159:GLN:HG2	2.03	0.58
1:F:136:THR:CG2	1:F:139:GLU:H	2.16	0.58
1:D:102:ARG:NH2	1:D:133:MET:O	2.35	0.58
1:F:78:GLU:HG2	4:F:2051:HOH:O	2.03	0.58
1:B:183:MET:O	1:B:210:ARG:HD2	2.03	0.58
1:G:100:THR:OG1	1:G:103:GLU:HG3	2.04	0.58
1:A:39:ARG:NH1	4:C:2057:HOH:O	2.36	0.58
1:A:78:GLU:OE1	1:C:34:ASN:HB3	2.02	0.58
1:D:100:THR:OG1	1:D:103:GLU:HG3	2.03	0.58
1:E:78:GLU:HB2	4:E:2038:HOH:O	2.04	0.58
1:E:206:ALA:O	1:E:209:LEU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:ARG:HD2	4:F:2112:HOH:O	2.02	0.57
1:H:137:GLN:HE21	1:H:148:ARG:HE	1.52	0.57
1:B:40:LYS:O	1:B:44:GLU:HG3	2.03	0.57
1:C:32:ARG:CZ	4:C:2004:HOH:O	2.51	0.57
1:E:212:ARG:NH2	4:E:2108:HOH:O	2.37	0.57
1:B:34:ASN:HD21	1:B:36:ARG:HH21	1.53	0.57
1:A:36:ARG:NH1	1:C:73:GLU:OE2	2.35	0.57
1:E:136:THR:HG22	1:E:138:GLU:H	1.70	0.57
1:G:102:ARG:HG3	1:G:102:ARG:HH21	1.69	0.57
1:D:34:ASN:ND2	1:D:36:ARG:H	2.03	0.57
1:G:136:THR:HB	1:G:139:GLU:HG3	1.86	0.56
1:G:34:ASN:HD21	1:G:36:ARG:HB2	1.69	0.56
1:D:177:HIS:HE1	1:D:201:LEU:O	1.88	0.56
1:H:195:GLU:O	1:H:199:LYS:HG2	2.06	0.56
1:D:40:LYS:O	1:D:44:GLU:HG3	2.05	0.56
1:E:212:ARG:HB3	4:E:2102:HOH:O	2.05	0.56
1:H:26:LEU:HD23	1:H:26:LEU:N	2.20	0.56
1:C:60:LEU:HD11	1:C:80:ARG:HD2	1.86	0.56
1:F:100:THR:OG1	1:F:103:GLU:HG3	2.06	0.56
1:B:195:GLU:OE1	1:B:199:LYS:HE2	2.04	0.56
1:D:45:GLU:O	1:D:49:GLU:HG3	2.06	0.56
1:E:24:VAL:HG12	1:E:25:ARG:N	2.20	0.56
1:A:100:THR:OG1	1:A:103:GLU:HG3	2.06	0.56
1:A:142:ARG:HE	1:A:142:ARG:CA	2.07	0.56
1:B:25:ARG:NH1	1:G:92:VAL:N	2.52	0.56
1:E:32:ARG:HH11	1:E:32:ARG:CB	2.17	0.56
1:D:141:ALA:HB1	1:D:146:LYS:O	2.06	0.56
1:E:91:GLU:HA	1:F:28:LEU:H	1.71	0.55
1:D:102:ARG:HG3	4:D:2049:HOH:O	2.05	0.55
1:D:39:ARG:HH22	1:H:117:ASP:CB	2.16	0.55
1:H:34:ASN:HD22	1:H:35:PRO:N	2.04	0.55
1:G:136:THR:HG22	1:G:137:GLN:N	2.21	0.55
1:C:34:ASN:ND2	1:C:36:ARG:NH2	2.55	0.55
1:G:24:VAL:CG1	1:G:25:ARG:H	2.19	0.55
1:A:59:LEU:HD22	1:A:80:ARG:CG	2.36	0.55
1:B:111:GLU:HB3	4:B:2061:HOH:O	2.06	0.55
1:G:32:ARG:HG2	4:G:2002:HOH:O	2.06	0.55
1:F:136:THR:HG22	1:F:139:GLU:CG	2.37	0.55
1:B:39:ARG:NH2	1:G:117:ASP:HB3	2.20	0.55
1:B:34:ASN:HD22	1:B:34:ASN:C	2.10	0.55
1:B:34:ASN:HB3	1:G:78:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ARG:HD3	1:H:105:LEU:HA	1.89	0.55
1:H:68:GLN:HA	1:H:68:GLN:NE2	2.22	0.54
1:C:59:LEU:HD23	1:C:60:LEU:HD23	1.89	0.54
1:H:59:LEU:HD22	1:H:80:ARG:HG2	1.88	0.54
1:B:24:VAL:HG12	1:B:25:ARG:N	2.21	0.54
1:D:204:ARG:NH2	1:D:205:GLN:HG2	2.23	0.54
1:F:102:ARG:HG2	4:F:2064:HOH:O	2.06	0.54
1:A:24:VAL:HG22	1:A:25:ARG:N	2.22	0.54
1:D:57:LYS:NZ	1:H:190:LEU:HD11	2.22	0.54
1:E:39:ARG:HH22	1:F:117:ASP:CB	2.20	0.54
1:E:36:ARG:NH1	1:F:73:GLU:OE2	2.40	0.54
1:B:74:LEU:HB3	1:G:34:ASN:HB2	1.90	0.54
1:C:40:LYS:O	1:C:44:GLU:HG3	2.07	0.54
1:D:61:GLN:HG2	1:D:80:ARG:NH1	2.23	0.54
1:E:68:GLN:NE2	1:E:68:GLN:HA	2.22	0.54
1:A:143:ARG:HH21	1:A:143:ARG:HG2	1.71	0.54
1:B:67:PRO:HG3	1:B:96:VAL:CG1	2.37	0.54
1:C:34:ASN:ND2	1:C:36:ARG:H	2.05	0.54
1:C:199:LYS:HB2	1:C:201:LEU:CD1	2.37	0.54
1:C:56:GLU:HB2	1:C:57:LYS:HD2	1.88	0.54
1:D:39:ARG:NH2	1:H:117:ASP:HB3	2.18	0.54
1:H:24:VAL:HG12	1:H:25:ARG:H	1.73	0.54
1:A:201:LEU:CB	1:A:205:GLN:HE21	2.20	0.53
1:B:209:LEU:C	4:B:2123:HOH:O	2.45	0.53
1:G:95:VAL:HG12	1:G:97:LYS:CD	2.38	0.53
1:H:59:LEU:HD22	1:H:80:ARG:CG	2.39	0.53
1:B:102:ARG:HG2	1:B:133:MET:HE3	1.91	0.53
1:E:34:ASN:HB3	1:F:78:GLU:OE1	2.08	0.53
1:G:78:GLU:O	1:G:82:ARG:HG3	2.08	0.53
1:G:200:GLY:C	1:G:202:SER:H	2.11	0.53
1:H:143:ARG:HH21	1:H:143:ARG:HG2	1.74	0.53
1:B:25:ARG:CB	1:B:25:ARG:CZ	2.85	0.53
1:D:41:ARG:O	1:D:45:GLU:HG3	2.09	0.53
1:E:72:TYR:CD2	1:F:26:LEU:HD23	2.43	0.53
1:A:34:ASN:HD22	1:A:34:ASN:C	2.11	0.52
1:B:138:GLU:O	1:B:142:ARG:HG3	2.09	0.52
1:H:34:ASN:C	1:H:34:ASN:HD22	2.12	0.52
1:B:24:VAL:CG1	1:B:25:ARG:N	2.72	0.52
1:C:136:THR:O	1:C:140:VAL:HG23	2.10	0.52
1:H:208:ALA:C	1:H:209:LEU:HD12	2.30	0.52
1:G:204:ARG:HH11	1:G:204:ARG:HG3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:VAL:CG1	1:G:25:ARG:N	2.70	0.52
1:G:131:LEU:HD11	1:G:155:LEU:HD11	1.90	0.52
1:E:210:ARG:HA	4:E:2105:HOH:O	2.10	0.52
1:A:117:ASP:CB	1:C:39:ARG:HH22	2.18	0.52
1:E:39:ARG:NH1	1:F:118:LEU:HD23	2.24	0.52
1:G:34:ASN:HD22	1:G:34:ASN:C	2.14	0.52
1:G:64:LEU:HD22	1:G:75:VAL:CB	2.33	0.52
1:B:137:GLN:HG3	4:B:2075:HOH:O	2.08	0.52
1:C:32:ARG:HH11	1:C:32:ARG:HG2	1.75	0.52
1:C:137:GLN:HE22	1:C:152:ALA:HB2	1.75	0.51
1:D:34:ASN:HB3	1:H:78:GLU:OE1	2.10	0.51
1:D:37:GLN:HB3	4:D:2018:HOH:O	2.11	0.51
1:A:34:ASN:HB3	1:C:78:GLU:OE1	2.10	0.51
1:F:48:LYS:NZ	1:F:55:ARG:HH22	2.08	0.51
1:B:34:ASN:HD22	1:B:36:ARG:H	1.57	0.51
4:E:2036:HOH:O	1:F:36:ARG:HD2	2.10	0.51
1:F:25:ARG:HG3	1:F:25:ARG:HH21	1.75	0.51
1:A:34:ASN:HD22	1:A:35:PRO:N	2.08	0.51
1:E:191:TRP:CZ3	1:E:213:LEU:HD12	2.45	0.51
1:A:136:THR:HG21	4:A:2102:HOH:O	2.10	0.51
1:C:102:ARG:NH1	1:C:133:MET:HB3	2.26	0.51
1:C:41:ARG:O	1:C:45:GLU:HG3	2.10	0.51
1:E:40:LYS:O	1:E:44:GLU:HG3	2.10	0.51
1:G:34:ASN:HD22	1:G:35:PRO:N	2.08	0.51
1:A:187:GLU:H	1:A:187:GLU:CD	2.13	0.51
1:E:211:GLU:O	1:E:213:LEU:N	2.44	0.51
1:E:44:GLU:O	1:E:48:LYS:HD3	2.11	0.51
1:E:54:ILE:HG22	1:E:89:LEU:HD11	1.93	0.51
1:B:102:ARG:NH2	1:B:133:MET:HE2	2.26	0.50
1:E:78:GLU:OE1	1:F:34:ASN:HB3	2.11	0.50
1:F:64:LEU:HD12	1:F:75:VAL:CB	2.39	0.50
1:H:27:PRO:HG2	1:H:30:SER:CB	2.41	0.50
1:C:143:ARG:HG3	1:C:143:ARG:HH11	1.76	0.50
1:E:34:ASN:HD22	1:E:35:PRO:N	2.10	0.50
1:F:195:GLU:O	1:F:199:LYS:HB2	2.11	0.50
1:A:50:LEU:HD13	1:A:83:ALA:CB	2.41	0.50
1:E:117:ASP:HB3	1:F:39:ARG:HH22	1.76	0.50
1:E:60:LEU:C	1:E:60:LEU:HD13	2.32	0.50
1:G:112:ASN:ND2	4:G:2075:HOH:O	2.44	0.50
1:D:202:SER:OG	1:D:205:GLN:HG3	2.11	0.50
1:A:179:ARG:HD3	4:A:2118:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:THR:HG22	1:D:139:GLU:CG	2.42	0.50
1:E:177:HIS:HE1	1:E:201:LEU:O	1.94	0.50
1:H:27:PRO:HG2	1:H:30:SER:HB3	1.94	0.50
1:A:142:ARG:NH2	1:H:55:ARG:NE	2.60	0.50
1:B:34:ASN:ND2	1:B:36:ARG:NH2	2.59	0.49
1:B:34:ASN:HD22	1:B:35:PRO:N	2.10	0.49
1:E:32:ARG:CG	1:E:32:ARG:HH11	2.25	0.49
1:E:94:ALA:HB3	1:F:26:LEU:HD13	1.94	0.49
1:A:204:ARG:HG3	1:A:204:ARG:NH2	2.27	0.49
1:C:60:LEU:HD11	1:C:80:ARG:HH11	1.77	0.49
1:A:28:LEU:HD23	1:A:28:LEU:O	2.13	0.49
1:F:48:LYS:HG2	1:F:86:MET:HE1	1.95	0.49
1:D:156:ARG:NH1	4:D:2077:HOH:O	2.44	0.49
1:E:163:GLU:H	1:E:163:GLU:CD	2.15	0.49
1:E:68:GLN:HE21	1:E:68:GLN:CA	2.22	0.49
1:G:194:LYS:HG3	4:G:2119:HOH:O	2.12	0.49
1:B:39:ARG:HH22	1:G:117:ASP:CB	2.20	0.49
1:F:26:LEU:HD12	1:F:26:LEU:N	2.28	0.49
1:F:41:ARG:O	1:F:45:GLU:HG3	2.12	0.49
1:A:117:ASP:HB3	1:C:39:ARG:NH2	2.20	0.49
1:C:27:PRO:HG2	1:C:30:SER:OG	2.13	0.49
1:C:170:ARG:HE	1:C:172:GLU:CD	2.16	0.49
1:B:95:VAL:HG22	1:G:23:VAL:HA	1.94	0.49
1:H:131:LEU:HD11	1:H:155:LEU:HD11	1.95	0.49
1:A:25:ARG:N	1:A:25:ARG:HD3	2.28	0.49
4:B:2114:HOH:O	1:G:60:LEU:HD11	2.12	0.49
1:A:26:LEU:HD21	1:C:94:ALA:HB3	1.95	0.49
1:E:141:ALA:HB1	1:E:146:LYS:O	2.13	0.49
1:A:142:ARG:HH21	1:H:55:ARG:HE	1.59	0.49
1:A:136:THR:HG23	1:A:138:GLU:H	1.77	0.48
1:G:68:GLN:HA	1:G:68:GLN:NE2	2.27	0.48
1:E:60:LEU:HD21	1:F:194:LYS:CG	2.42	0.48
1:E:95:VAL:HG22	1:F:23:VAL:HA	1.94	0.48
1:G:175:ALA:O	1:G:179:ARG:HG3	2.13	0.48
1:B:57:LYS:HE3	4:G:2107:HOH:O	2.13	0.48
1:D:177:HIS:CE1	1:D:201:LEU:O	2.65	0.48
1:C:113:LEU:HD23	1:C:118:LEU:HD11	1.94	0.48
1:E:209:LEU:HA	4:E:2102:HOH:O	2.14	0.48
1:E:25:ARG:NH2	1:E:25:ARG:HG3	2.27	0.48
1:F:102:ARG:NE	1:F:102:ARG:HA	2.28	0.48
1:G:201:LEU:H	1:G:201:LEU:HD23	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD21	1:C:85:LEU:HD23	1.92	0.48
1:C:138:GLU:N	1:C:138:GLU:OE1	2.45	0.48
1:C:156:ARG:HH21	1:C:156:ARG:HG2	1.78	0.48
1:F:141:ALA:HB1	1:F:146:LYS:O	2.13	0.48
1:G:34:ASN:HD22	1:G:36:ARG:H	1.58	0.48
4:F:2087:HOH:O	1:G:55:ARG:HD3	2.13	0.48
1:A:136:THR:HG22	1:A:139:GLU:N	2.23	0.48
1:C:204:ARG:HD3	4:C:2108:HOH:O	2.14	0.48
1:A:142:ARG:NH1	4:A:2111:HOH:O	2.47	0.47
1:A:27:PRO:HA	1:C:91:GLU:HG2	1.96	0.47
1:B:156:ARG:HG2	1:B:156:ARG:HH21	1.79	0.47
1:B:25:ARG:NE	1:B:25:ARG:HA	2.29	0.47
1:A:26:LEU:HD12	1:C:92:VAL:O	2.15	0.47
1:G:168:LEU:HD21	4:G:2112:HOH:O	2.13	0.47
1:H:136:THR:CG2	1:H:139:GLU:H	2.27	0.47
1:A:105:LEU:HA	1:C:36:ARG:HD3	1.96	0.47
1:B:25:ARG:HH11	1:G:92:VAL:CA	2.28	0.47
1:D:68:GLN:NE2	1:D:68:GLN:HA	2.29	0.47
1:F:24:VAL:CG1	1:F:25:ARG:H	2.20	0.47
1:G:141:ALA:HB1	1:G:146:LYS:O	2.14	0.47
1:D:212:ARG:HH21	1:D:212:ARG:CB	2.27	0.47
1:G:120:PRO:HG3	4:G:2112:HOH:O	2.13	0.47
1:C:57:LYS:HD2	1:C:57:LYS:H	1.80	0.47
1:G:199:LYS:O	1:G:203:VAL:HG23	2.15	0.47
1:D:56:GLU:C	1:D:57:LYS:HG3	2.34	0.47
1:E:32:ARG:HB2	1:E:33:PRO:HD2	1.96	0.47
1:C:68:GLN:HG3	1:C:73:GLU:HB2	1.97	0.47
1:D:34:ASN:C	1:D:34:ASN:HD22	2.17	0.47
1:H:204:ARG:HG3	1:H:204:ARG:HH21	1.80	0.47
1:A:142:ARG:CZ	4:A:2111:HOH:O	2.62	0.47
1:B:210:ARG:NH2	4:B:2127:HOH:O	2.48	0.47
1:E:34:ASN:HD22	1:E:34:ASN:C	2.18	0.47
1:C:61:GLN:OE1	1:C:61:GLN:HA	2.15	0.47
1:D:60:LEU:C	1:D:60:LEU:HD23	2.35	0.47
1:E:39:ARG:NH2	1:F:117:ASP:HB3	2.25	0.47
1:C:138:GLU:O	1:C:142:ARG:HG3	2.15	0.47
1:D:131:LEU:HD11	1:D:155:LEU:HD11	1.96	0.47
1:A:34:ASN:HD22	1:A:36:ARG:H	1.63	0.46
1:B:213:LEU:HD23	4:B:2128:HOH:O	2.14	0.46
1:D:156:ARG:HH21	1:D:156:ARG:HG2	1.79	0.46
1:E:136:THR:HG22	1:E:137:GLN:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ALA:HB1	1:A:146:LYS:O	2.15	0.46
1:C:78:GLU:HB2	4:C:2033:HOH:O	2.16	0.46
1:D:142:ARG:HD2	1:D:143:ARG:NH2	2.31	0.46
1:B:43:ALA:O	1:B:79:ARG:NH2	2.49	0.46
1:E:212:ARG:CG	1:E:212:ARG:O	2.63	0.46
1:B:85:LEU:HD23	1:G:28:LEU:HD21	1.97	0.46
1:D:104:ALA:HB1	1:H:36:ARG:NE	2.31	0.46
1:C:57:LYS:HD2	1:C:57:LYS:N	2.31	0.46
1:B:197:LEU:HD12	4:B:2114:HOH:O	2.16	0.46
1:F:156:ARG:HG2	1:F:156:ARG:HH21	1.81	0.46
1:H:163:GLU:CD	1:H:163:GLU:H	2.18	0.46
1:B:184:LEU:HD23	1:B:210:ARG:HG3	1.98	0.46
1:B:64:LEU:HD22	1:B:75:VAL:HB	1.98	0.46
1:A:39:ARG:HH22	1:C:117:ASP:HB3	1.81	0.46
1:C:59:LEU:HD21	1:C:80:ARG:HG3	1.98	0.46
1:E:137:GLN:HE22	1:E:152:ALA:HB2	1.81	0.46
1:F:26:LEU:N	1:F:26:LEU:CD1	2.79	0.46
1:G:163:GLU:CD	1:G:163:GLU:H	2.19	0.46
1:B:91:GLU:HA	1:G:28:LEU:H	1.81	0.46
1:B:136:THR:H	1:B:139:GLU:CD	2.19	0.45
1:C:140:VAL:O	1:C:144:VAL:HG22	2.16	0.45
1:B:56:GLU:OE2	1:B:56:GLU:N	2.49	0.45
1:D:34:ASN:HD22	1:D:35:PRO:N	2.14	0.45
1:F:34:ASN:HD22	1:F:35:PRO:N	2.14	0.45
1:C:210:ARG:O	1:C:211:GLU:HB3	2.16	0.45
1:E:61:GLN:HB3	1:E:61:GLN:HE21	1.51	0.45
1:B:102:ARG:O	1:B:133:MET:HE1	2.16	0.45
1:C:60:LEU:H	1:C:60:LEU:CD2	2.21	0.45
1:E:39:ARG:HH12	1:F:118:LEU:HD23	1.82	0.45
1:B:167:ALA:HA	1:B:170:ARG:NH2	2.31	0.45
1:F:163:GLU:H	1:F:163:GLU:CD	2.21	0.45
1:E:193:LEU:HD13	1:F:60:LEU:CD2	2.47	0.45
1:H:34:ASN:HD22	1:H:36:ARG:H	1.64	0.45
1:D:163:GLU:CD	1:D:163:GLU:H	2.18	0.44
1:D:194:LYS:HD3	4:D:2107:HOH:O	2.17	0.44
1:H:136:THR:CG2	1:H:139:GLU:HG3	2.47	0.44
1:B:163:GLU:CD	1:B:163:GLU:H	2.19	0.44
1:C:117:ASP:HB3	4:C:2057:HOH:O	2.17	0.44
1:H:24:VAL:CG1	1:H:25:ARG:N	2.77	0.44
1:G:156:ARG:HH21	1:G:156:ARG:HG2	1.82	0.44
1:H:199:LYS:HG3	1:H:201:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:GLU:HG2	4:B:2073:HOH:O	2.18	0.44
1:C:32:ARG:NH2	4:C:2004:HOH:O	2.49	0.44
1:G:200:GLY:C	1:G:202:SER:N	2.71	0.44
1:B:206:ALA:O	1:B:209:LEU:HB2	2.17	0.44
1:B:36:ARG:HD3	1:G:105:LEU:HA	2.00	0.44
1:A:32:ARG:HH11	1:C:68:GLN:HE21	1.64	0.44
1:E:36:ARG:HD2	4:F:2067:HOH:O	2.18	0.44
1:A:85:LEU:CD2	1:C:28:LEU:HG	2.48	0.44
1:D:74:LEU:HB3	1:H:34:ASN:HB2	1.99	0.44
1:F:143:ARG:HG2	1:F:143:ARG:HH21	1.83	0.44
1:D:142:ARG:HG3	1:D:143:ARG:N	2.33	0.44
1:G:97:LYS:HB2	1:G:97:LYS:HE2	1.80	0.44
1:C:60:LEU:CG	1:C:80:ARG:HD2	2.48	0.43
1:D:68:GLN:CG	1:H:32:ARG:NH2	2.79	0.43
1:G:174:THR:N	1:G:177:HIS:HD2	1.98	0.43
1:B:61:GLN:NE2	1:G:197:LEU:HD13	2.33	0.43
1:E:211:GLU:C	1:E:213:LEU:N	2.71	0.43
1:G:64:LEU:HD23	1:G:65:VAL:N	2.32	0.43
1:A:201:LEU:HB3	1:A:205:GLN:HE21	1.82	0.43
1:E:193:LEU:HD13	1:F:60:LEU:HD21	1.99	0.43
1:H:34:ASN:HD22	1:H:35:PRO:CD	2.30	0.43
1:C:202:SER:H	1:C:205:GLN:CD	2.20	0.43
1:F:86:MET:HG3	4:F:2027:HOH:O	2.17	0.43
1:G:133:MET:HE2	4:G:2069:HOH:O	2.18	0.43
1:B:137:GLN:HE22	1:B:152:ALA:HB2	1.82	0.43
1:A:131:LEU:HD11	1:A:155:LEU:HD11	2.01	0.43
1:D:25:ARG:NH1	4:H:2062:HOH:O	2.52	0.43
1:E:34:ASN:HD22	1:E:36:ARG:H	1.62	0.43
1:F:203:VAL:O	1:F:207:GLU:HG3	2.18	0.43
1:G:118:LEU:HD22	1:G:122:GLU:HB3	2.00	0.43
1:C:60:LEU:HB2	4:C:2025:HOH:O	2.17	0.43
1:D:175:ALA:O	1:D:179:ARG:HG3	2.19	0.43
1:E:137:GLN:HE21	1:E:148:ARG:HD3	1.84	0.43
1:F:184:LEU:HD21	1:F:209:LEU:HB3	2.00	0.43
1:G:186:PRO:HA	1:G:189:ARG:HD2	2.00	0.43
1:H:156:ARG:HG2	1:H:156:ARG:HH21	1.84	0.43
1:A:64:LEU:HD23	1:A:65:VAL:N	2.33	0.43
1:C:177:HIS:HE1	1:C:201:LEU:O	2.02	0.43
1:A:136:THR:CG2	1:A:138:GLU:H	2.32	0.43
1:C:41:ARG:HA	1:C:41:ARG:HD3	1.79	0.43
1:E:24:VAL:CG1	1:E:25:ARG:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:ARG:C	1:H:26:LEU:HD23	2.40	0.42
1:B:54:ILE:HD11	1:B:83:ALA:C	2.39	0.42
1:A:34:ASN:HB2	1:C:74:LEU:HB3	2.01	0.42
1:C:60:LEU:CD1	1:C:80:ARG:HD2	2.49	0.42
1:E:143:ARG:HH21	1:E:143:ARG:HG3	1.83	0.42
1:E:67:PRO:HG2	1:E:98:ASP:OD2	2.19	0.42
1:F:34:ASN:C	1:F:34:ASN:HD22	2.21	0.42
1:G:118:LEU:HD22	1:G:122:GLU:CB	2.50	0.42
1:B:25:ARG:HH11	1:G:92:VAL:N	2.16	0.42
1:B:45:GLU:O	1:B:49:GLU:HG3	2.20	0.42
1:B:55:ARG:HA	1:B:87:ALA:HB1	2.01	0.42
1:D:90:GLN:HA	1:D:90:GLN:HE21	1.84	0.42
1:G:45:GLU:HB3	4:G:2021:HOH:O	2.18	0.42
1:D:57:LYS:NZ	1:H:190:LEU:CD1	2.83	0.42
1:C:102:ARG:HH11	1:C:102:ARG:HG3	1.83	0.42
1:F:175:ALA:O	1:F:179:ARG:HG3	2.19	0.42
4:D:2036:HOH:O	1:H:36:ARG:HD2	2.19	0.42
1:A:41:ARG:HD3	1:A:41:ARG:HA	1.80	0.42
1:D:143:ARG:HH21	1:D:143:ARG:HG2	1.84	0.42
1:E:32:ARG:NH1	4:E:2006:HOH:O	2.53	0.42
1:D:90:GLN:HA	1:D:90:GLN:NE2	2.34	0.42
1:E:45:GLU:O	1:E:49:GLU:HG3	2.20	0.42
1:C:110:VAL:HG11	1:C:143:ARG:HD2	2.01	0.42
1:C:52:ASP:HA	1:C:55:ARG:HH21	1.84	0.42
1:G:204:ARG:HG3	1:G:204:ARG:NH1	2.35	0.42
1:B:136:THR:HG22	1:B:137:GLN:N	2.35	0.41
1:B:25:ARG:HH12	1:G:91:GLU:C	2.23	0.41
1:D:212:ARG:HH21	1:D:212:ARG:HB2	1.83	0.41
1:E:40:LYS:HG3	4:E:2014:HOH:O	2.20	0.41
1:H:166:GLU:HB3	4:H:2109:HOH:O	2.20	0.41
1:H:25:ARG:CB	1:H:25:ARG:HH21	2.21	0.41
1:A:100:THR:HG23	1:A:103:GLU:OE2	2.20	0.41
1:C:205:GLN:H	1:C:205:GLN:HG2	1.71	0.41
1:A:156:ARG:HG2	1:A:156:ARG:HH21	1.84	0.41
1:A:26:LEU:HD11	1:A:31:ILE:HD11	2.02	0.41
1:B:136:THR:O	1:B:140:VAL:HG23	2.20	0.41
1:E:34:ASN:HD22	1:E:35:PRO:CD	2.34	0.41
1:G:25:ARG:HG3	1:G:25:ARG:HH21	1.85	0.41
1:A:201:LEU:CB	1:A:205:GLN:NE2	2.84	0.41
1:A:136:THR:HG21	1:A:138:GLU:HB3	2.00	0.41
1:C:52:ASP:HA	1:C:55:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ILE:CD1	1:C:84:ALA:HA	2.51	0.41
1:G:78:GLU:OE2	1:G:82:ARG:NH1	2.54	0.41
1:A:207:GLU:O	1:A:208:ALA:HB2	2.21	0.41
1:G:187:GLU:CD	1:G:187:GLU:H	2.23	0.41
1:G:41:ARG:O	1:G:45:GLU:HG3	2.20	0.41
1:H:204:ARG:HG3	1:H:204:ARG:NH2	2.35	0.41
1:A:73:GLU:OE2	1:C:36:ARG:NH1	2.46	0.41
1:C:100:THR:OG1	1:C:103:GLU:HG3	2.20	0.41
1:C:202:SER:N	1:C:205:GLN:CG	2.82	0.41
1:D:64:LEU:C	1:D:64:LEU:HD23	2.41	0.41
1:F:48:LYS:HE2	1:F:86:MET:CE	2.51	0.41
1:H:187:GLU:H	1:H:187:GLU:CD	2.24	0.41
1:H:202:SER:H	1:H:205:GLN:HE21	1.66	0.41
1:B:102:ARG:HG2	1:B:133:MET:CE	2.51	0.41
1:F:131:LEU:HD11	1:F:155:LEU:HD11	2.02	0.41
1:B:40:LYS:HG3	4:B:2014:HOH:O	2.20	0.41
1:B:65:VAL:HG12	1:B:74:LEU:HA	2.03	0.41
1:C:110:VAL:HG12	1:C:114:GLN:HE21	1.86	0.41
1:F:137:GLN:HE21	1:F:148:ARG:HE	1.69	0.41
1:H:112:ASN:ND2	4:H:2081:HOH:O	2.53	0.40
1:H:190:LEU:HA	1:H:190:LEU:HD23	1.89	0.40
1:A:61:GLN:NE2	4:A:2038:HOH:O	2.54	0.40
1:C:59:LEU:CD2	1:C:60:LEU:HD23	2.50	0.40
1:H:96:VAL:O	1:H:97:LYS:HD2	2.21	0.40
1:A:201:LEU:HB2	1:A:205:GLN:HE21	1.86	0.40
1:D:36:ARG:HH11	1:H:66:ARG:NH1	2.20	0.40
1:F:82:ARG:HH21	1:F:82:ARG:HG2	1.87	0.40
1:B:170:ARG:NH2	1:B:172:GLU:CD	2.75	0.40
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.83	0.40
1:D:61:GLN:HA	1:D:62:PRO:HD3	1.92	0.40
1:F:186:PRO:HA	1:F:189:ARG:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	185/230 (80%)	183 (99%)	0	2 (1%)	14	15
1	B	191/230 (83%)	186 (97%)	5 (3%)	0	100	100
1	C	188/230 (82%)	185 (98%)	2 (1%)	1 (0%)	29	35
1	D	191/230 (83%)	188 (98%)	3 (2%)	0	100	100
1	E	190/230 (83%)	186 (98%)	3 (2%)	1 (0%)	29	35
1	F	187/230 (81%)	181 (97%)	6 (3%)	0	100	100
1	G	185/230 (80%)	178 (96%)	7 (4%)	0	100	100
1	H	186/230 (81%)	182 (98%)	4 (2%)	0	100	100
All	All	1503/1840 (82%)	1469 (98%)	30 (2%)	4 (0%)	41	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	212	ARG
1	A	208	ALA
1	C	60	LEU
1	A	207	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/184 (82%)	134 (89%)	17 (11%)	6	6
1	B	156/184 (85%)	140 (90%)	16 (10%)	7	8
1	C	154/184 (84%)	141 (92%)	13 (8%)	11	13
1	D	156/184 (85%)	147 (94%)	9 (6%)	20	27
1	E	156/184 (85%)	139 (89%)	17 (11%)	6	7
1	F	153/184 (83%)	141 (92%)	12 (8%)	12	16
1	G	151/184 (82%)	141 (93%)	10 (7%)	16	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	152/184 (83%)	139 (91%)	13 (9%)	10	12
All	All	1229/1472 (84%)	1122 (91%)	107 (9%)	10	12

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	26	LEU
1	A	34	ASN
1	A	41	ARG
1	A	47	LEU
1	A	50	LEU
1	A	64	LEU
1	A	74	LEU
1	A	105	LEU
1	A	117	ASP
1	A	136	THR
1	A	142	ARG
1	A	143	ARG
1	A	168	LEU
1	A	187	GLU
1	A	193	LEU
1	A	201	LEU
1	B	25	ARG
1	B	28	LEU
1	B	34	ASN
1	B	41	ARG
1	B	47	LEU
1	B	50	LEU
1	B	68	GLN
1	B	74	LEU
1	B	80	ARG
1	B	102	ARG
1	B	105	LEU
1	B	143	ARG
1	B	168	LEU
1	B	170	ARG
1	B	193	LEU
1	B	204	ARG
1	C	34	ASN
1	C	41	ARG
1	C	47	LEU

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Mol	Chain	Res	Type
1	C	50	LEU
1	C	57	LYS
1	C	60	LEU
1	C	74	LEU
1	C	105	LEU
1	C	118	LEU
1	C	143	ARG
1	C	168	LEU
1	C	193	LEU
1	C	205	GLN
1	D	34	ASN
1	D	41	ARG
1	D	50	LEU
1	D	68	GLN
1	D	74	LEU
1	D	105	LEU
1	D	168	LEU
1	D	193	LEU
1	D	212	ARG
1	E	28	LEU
1	E	32	ARG
1	E	34	ASN
1	E	41	ARG
1	E	47	LEU
1	E	50	LEU
1	E	61	GLN
1	E	68	GLN
1	E	74	LEU
1	E	105	LEU
1	E	114	GLN
1	E	143	ARG
1	E	148	ARG
1	E	168	LEU
1	E	193	LEU
1	E	204	ARG
1	E	209	LEU
1	F	26	LEU
1	F	34	ASN
1	F	41	ARG
1	F	47	LEU
1	F	48	LYS
1	F	50	LEU

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Mol	Chain	Res	Type
1	F	74	LEU
1	F	105	LEU
1	F	117	ASP
1	F	168	LEU
1	F	193	LEU
1	F	210	ARG
1	G	34	ASN
1	G	41	ARG
1	G	47	LEU
1	G	50	LEU
1	G	60	LEU
1	G	74	LEU
1	G	105	LEU
1	G	117	ASP
1	G	168	LEU
1	G	193	LEU
1	H	25	ARG
1	H	26	LEU
1	H	34	ASN
1	H	41	ARG
1	H	47	LEU
1	H	50	LEU
1	H	64	LEU
1	H	74	LEU
1	H	105	LEU
1	H	117	ASP
1	H	168	LEU
1	H	193	LEU
1	H	201	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	61	GLN
1	A	68	GLN
1	A	90	GLN
1	A	112	ASN
1	A	137	GLN
1	A	159	GLN
1	A	177	HIS
1	A	205	GLN

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Mol	Chain	Res	Type
1	B	34	ASN
1	B	90	GLN
1	B	114	GLN
1	B	137	GLN
1	B	159	GLN
1	B	177	HIS
1	B	205	GLN
1	C	34	ASN
1	C	114	GLN
1	C	137	GLN
1	C	177	HIS
1	D	34	ASN
1	D	90	GLN
1	D	114	GLN
1	D	137	GLN
1	D	177	HIS
1	D	205	GLN
1	E	34	ASN
1	E	61	GLN
1	E	68	GLN
1	E	137	GLN
1	E	177	HIS
1	F	34	ASN
1	F	61	GLN
1	F	68	GLN
1	F	90	GLN
1	F	114	GLN
1	F	137	GLN
1	F	177	HIS
1	G	34	ASN
1	G	61	GLN
1	G	68	GLN
1	G	90	GLN
1	G	112	ASN
1	G	137	GLN
1	G	159	GLN
1	G	177	HIS
1	H	34	ASN
1	H	61	GLN
1	H	68	GLN
1	H	90	GLN
1	H	137	GLN

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Mol	Chain	Res	Type
1	H	177	HIS
1	H	205	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 15 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 (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	187/230 (81%)	0.17	8 (4%)	35	42	15, 32, 69, 88	0
1	B	193/230 (83%)	0.37	13 (6%)	17	23	16, 37, 71, 95	0
1	C	190/230 (82%)	0.30	8 (4%)	36	43	15, 37, 67, 80	0
1	D	193/230 (83%)	0.39	12 (6%)	20	26	15, 38, 71, 84	0
1	E	192/230 (83%)	0.41	17 (8%)	9	13	17, 38, 74, 87	0
1	F	189/230 (82%)	0.18	4 (2%)	63	70	14, 33, 75, 101	0
1	G	187/230 (81%)	0.42	18 (9%)	8	10	17, 33, 77, 120	0
1	H	188/230 (81%)	0.26	10 (5%)	26	33	16, 33, 76, 93	0
All	All	1519/1840 (82%)	0.31	90 (5%)	22	28	14, 35, 73, 120	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	175	ALA	9.2
1	C	142	ARG	5.5
1	G	206	ALA	4.7
1	H	204	ARG	4.6
1	D	142	ARG	4.3
1	G	201	LEU	4.2
1	G	179	ARG	4.1
1	B	25	ARG	3.9
1	B	142	ARG	3.7
1	A	191	TRP	3.6
1	G	209	LEU	3.6
1	D	71	GLY	3.4
1	C	60	LEU	3.4
1	G	174	THR	3.3
1	E	96	VAL	3.3
1	D	144	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	71	GLY	3.2
1	G	196	ILE	3.1
1	D	139	GLU	3.1
1	A	204	ARG	3.1
1	B	69	GLY	3.1
1	E	70	ASP	3.0
1	B	70	ASP	3.0
1	E	69	GLY	3.0
1	H	200	GLY	2.9
1	A	187	GLU	2.9
1	D	94	ALA	2.9
1	C	61	GLN	2.8
1	E	149	SER	2.8
1	E	95	VAL	2.7
1	B	144	VAL	2.7
1	G	204	ARG	2.7
1	D	146	LYS	2.7
1	H	191	TRP	2.6
1	G	178	ALA	2.6
1	D	70	ASP	2.6
1	D	148	ARG	2.6
1	E	94	ALA	2.6
1	H	30	SER	2.6
1	E	90	GLN	2.6
1	C	95	VAL	2.6
1	G	176	GLY	2.6
1	A	209	LEU	2.5
1	G	205	GLN	2.5
1	B	215	MET	2.5
1	G	197	LEU	2.5
1	F	210	ARG	2.5
1	A	200	GLY	2.5
1	A	197	LEU	2.5
1	G	202	SER	2.4
1	H	23	VAL	2.4
1	D	91	GLU	2.4
1	E	211	GLU	2.4
1	E	59	LEU	2.3
1	E	92	VAL	2.3
1	G	203	VAL	2.3
1	E	143	ARG	2.3
1	H	187	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	143	ARG	2.3
1	E	54	ILE	2.3
1	E	98	ASP	2.3
1	F	211	GLU	2.3
1	B	212	ARG	2.3
1	D	149	SER	2.3
1	G	177	HIS	2.3
1	G	207	GLU	2.2
1	B	71	GLY	2.2
1	E	134	GLY	2.2
1	F	28	LEU	2.2
1	E	212	ARG	2.2
1	H	203	VAL	2.2
1	A	26	LEU	2.2
1	F	208	ALA	2.2
1	B	96	VAL	2.1
1	E	138	GLU	2.1
1	E	57	LYS	2.1
1	B	209	LEU	2.1
1	C	96	VAL	2.1
1	B	143	ARG	2.1
1	B	136	THR	2.1
1	H	197	LEU	2.1
1	H	188	ASP	2.1
1	A	183	MET	2.1
1	D	138	GLU	2.0
1	G	173	ILE	2.0
1	G	208	ALA	2.0
1	C	98	ASP	2.0
1	H	24	VAL	2.0
1	B	148	ARG	2.0
1	C	92	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 carbohydrates 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($Å^2$)	Q<0.9
3	MG	D	1217	1/1	0.91	0.45	27,27,27,27	0
3	MG	C	1214	1/1	0.94	0.43	24,24,24,24	0
2	CO	H	1210	1/1	0.97	0.21	64,64,64,64	0
2	CO	A	1211	1/1	0.97	0.22	56,56,56,56	0
2	CO	A	1209	1/1	0.97	0.12	46,46,46,46	0
2	CO	G	1209	1/1	0.98	0.22	61,61,61,61	0
2	CO	E	1215	1/1	0.98	0.16	52,52,52,52	0
2	CO	B	1215	1/1	0.99	0.11	33,33,33,33	0
2	CO	E	1214	1/1	0.99	0.10	34,34,34,34	0
2	CO	B	1216	1/1	0.99	0.17	24,24,24,24	0
2	CO	C	1213	1/1	0.99	0.08	34,34,34,34	0
2	CO	D	1215	1/1	0.99	0.08	26,26,26,26	0
2	CO	C	1212	1/1	1.00	0.14	23,23,23,23	0
2	CO	A	1210	1/1	1.00	0.15	22,22,22,22	0
2	CO	D	1216	1/1	1.00	0.15	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.