Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:46 AM GMT

PDB ID	:	2E6G
Title	:	Crystal structure of the stationary phase survival protein SurE from Thermus thermophilus HB8 in complex with phosphate
Authors	:	Iwasaki, W.; Miki, K.
Deposited on	:	2006-12-26
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

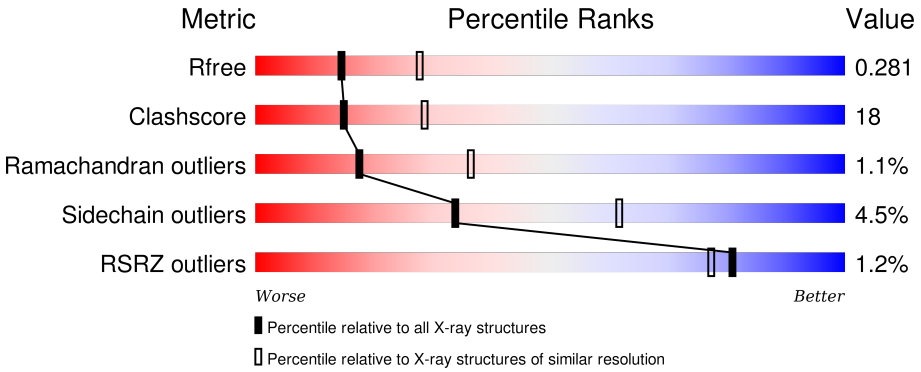
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	244	60% 27% • 9%
1	B	244	2% 61% 29% • 8%
1	C	244	2% 57% 33% • 8%
1	D	244	% 64% 27% • 7%
1	E	244	69% 25% • 5%

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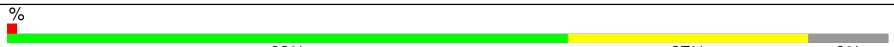
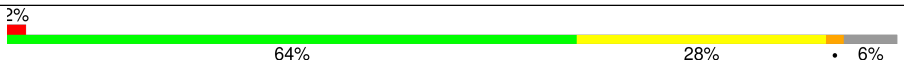
Mol	Chain	Length	Quality of chain
1	F	244	
1	G	244	
1	H	244	
1	I	244	
1	J	244	
1	K	244	
1	L	244	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	J	1202	-	-	X	-

2 Entry composition

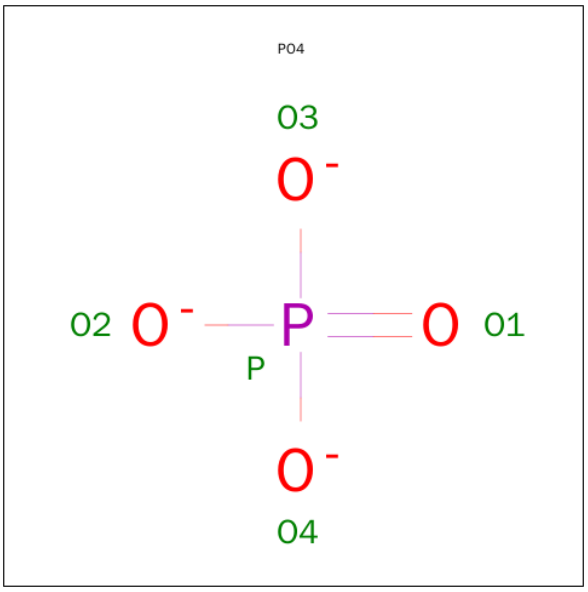
There are 3 unique types of molecules in this entry. The entry contains 21357 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5'-nucleotidase surE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1715	1113	299	300	3			
1	B	225	Total	C	N	O	S	0	0	0
			1749	1137	306	303	3			
1	C	225	Total	C	N	O	S	0	0	0
			1749	1136	304	306	3			
1	D	228	Total	C	N	O	S	0	0	0
			1772	1151	309	309	3			
1	E	233	Total	C	N	O	S	0	0	0
			1807	1170	315	319	3			
1	F	228	Total	C	N	O	S	0	0	0
			1770	1148	308	311	3			
1	G	229	Total	C	N	O	S	0	0	0
			1779	1155	310	311	3			
1	H	229	Total	C	N	O	S	0	0	0
			1780	1154	310	313	3			
1	I	227	Total	C	N	O	S	0	0	0
			1763	1144	307	309	3			
1	J	222	Total	C	N	O	S	0	0	0
			1726	1120	301	302	3			
1	K	226	Total	C	N	O	S	0	0	0
			1756	1140	305	308	3			
1	L	229	Total	C	N	O	S	0	0	0
			1780	1154	311	312	3			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	3	Total O 3 3	0	0
3	C	3	Total O 3 3	0	0
3	D	3	Total O 3 3	0	0
3	E	8	Total O 8 8	0	0
3	F	9	Total O 9 9	0	0
3	G	3	Total O 3 3	0	0
3	H	4	Total O 4 4	0	0

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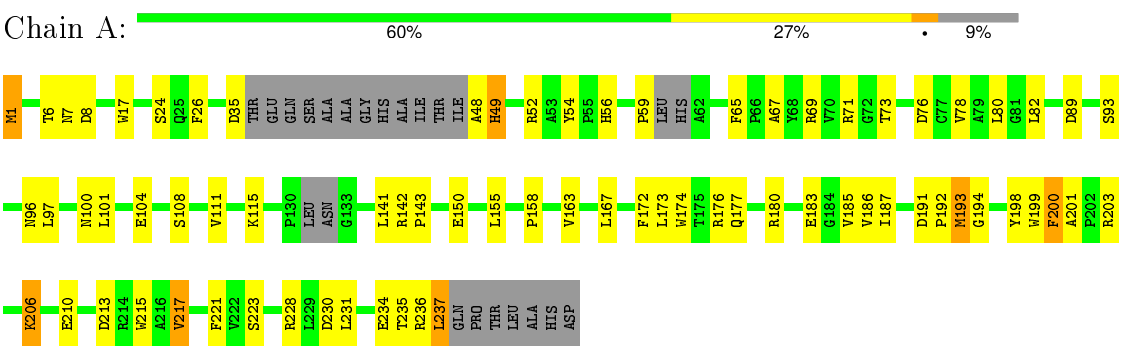
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	12	Total O 12 12	0	0
3	J	7	Total O 7 7	0	0
3	K	12	Total O 12 12	0	0
3	L	12	Total O 12 12	0	0

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 errors 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.

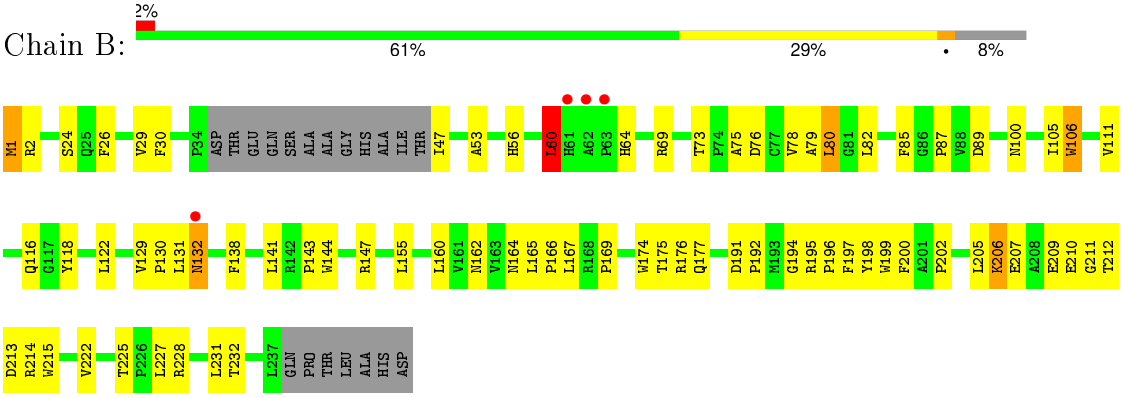
- Molecule 1: 5'-nucleotidase surE

Chain A:



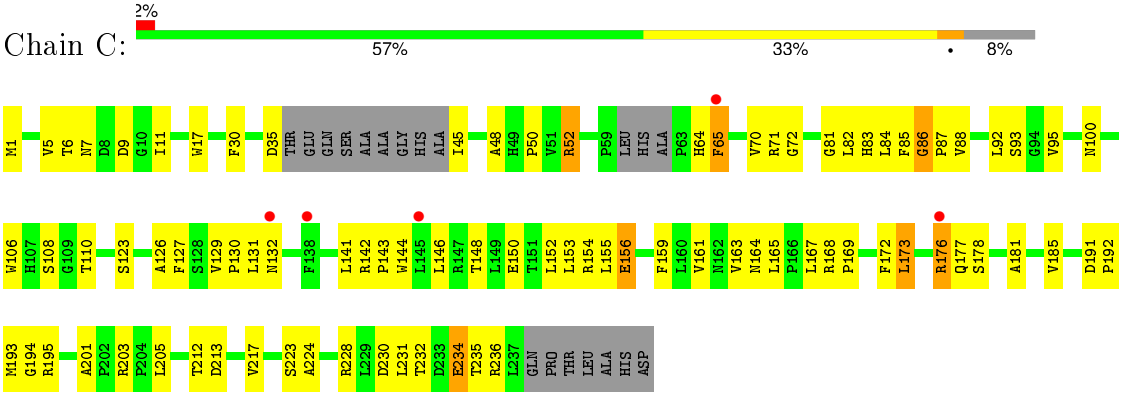
- Molecule 1: 5'-nucleotidase surE

Chain B:



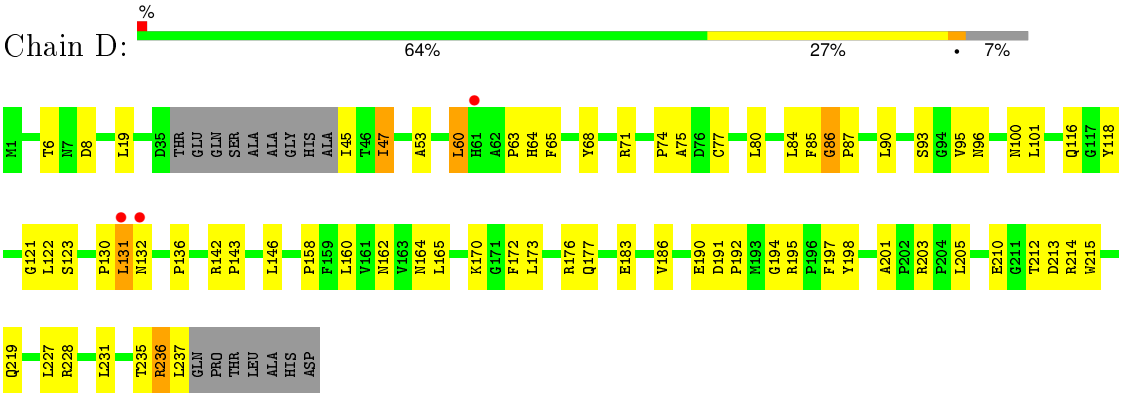
- Molecule 1: 5'-nucleotidase surE

Chain C:



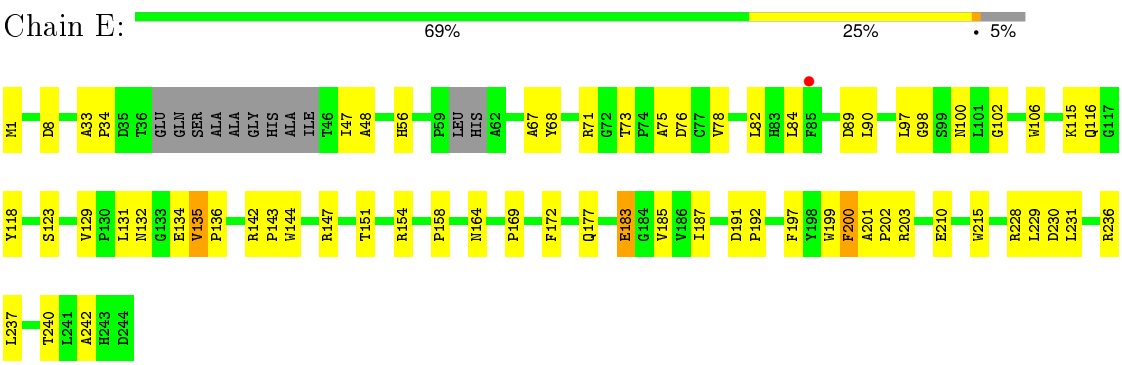
• Molecule 1: 5'-nucleotidase surE

Chain D:



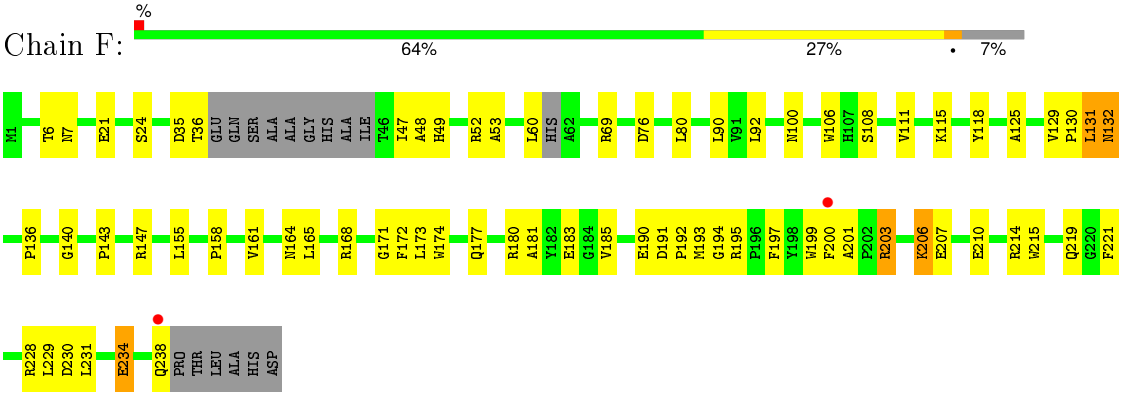
• Molecule 1: 5'-nucleotidase surE

Chain E:



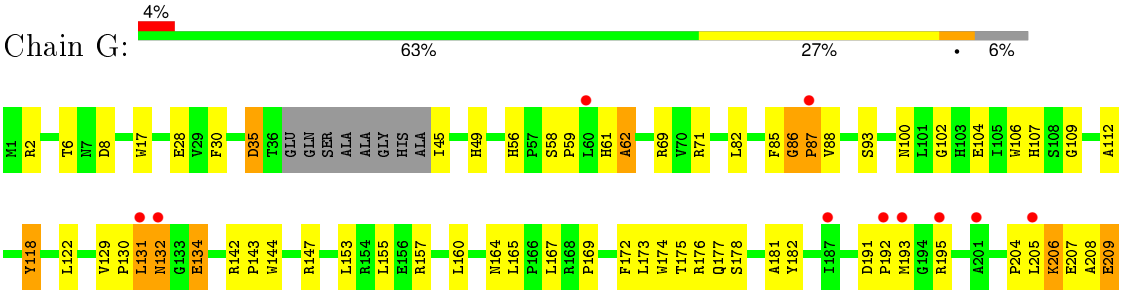
• Molecule 1: 5'-nucleotidase surE

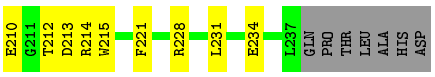
Chain F:



• Molecule 1: 5'-nucleotidase surE

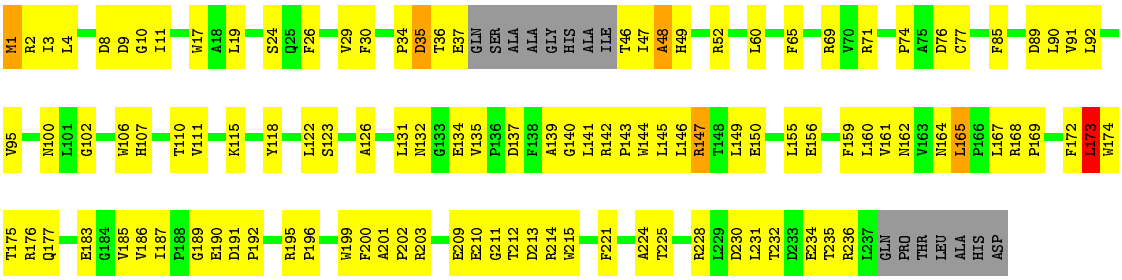
Chain G:





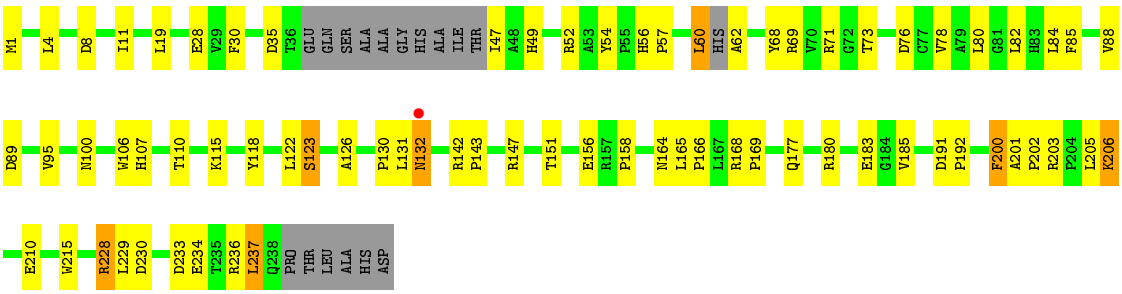
- Molecule 1: 5'-nucleotidase surE

Chain H:



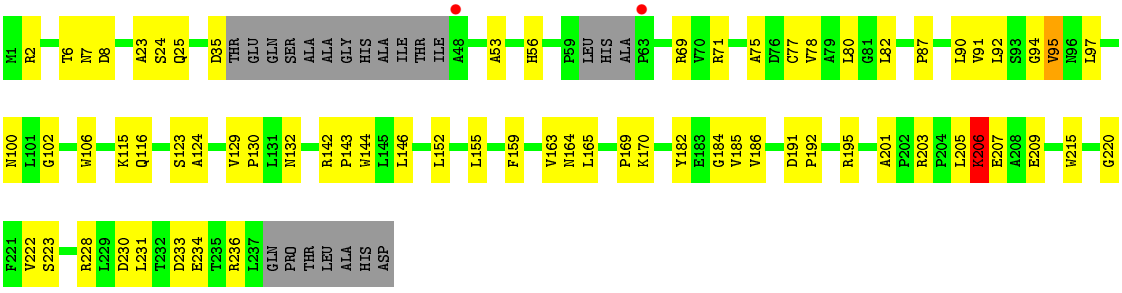
- Molecule 1: 5'-nucleotidase surE

Chain I:



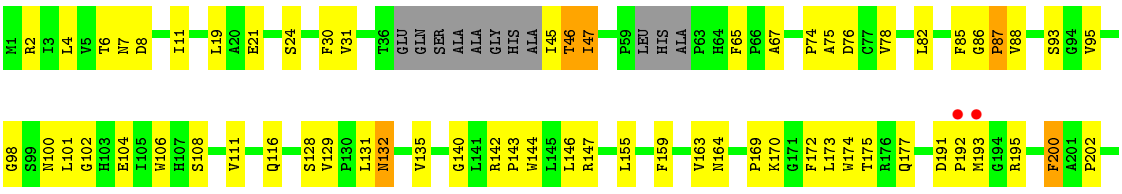
- Molecule 1: 5'-nucleotidase surE

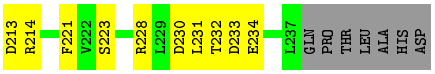
Chain J:



- Molecule 1: 5'-nucleotidase surE

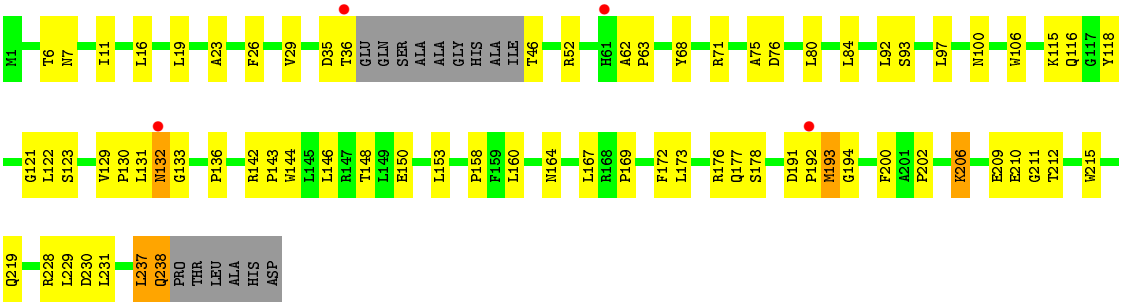
Chain K:





• Molecule 1: 5'-nucleotidase surE

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.64Å 196.08Å 253.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.53 – 2.60 45.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.53-2.60) 99.8 (45.53-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.27 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.284 0.218 , 0.281	Depositor DCC
R_{free} test set	4728 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 94430 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21357	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.47	0/1769	0.69	0/2419
1	B	0.47	0/1806	0.70	0/2473
1	C	0.46	0/1804	0.70	0/2468
1	D	0.49	0/1829	0.70	0/2505
1	E	0.52	0/1864	0.71	0/2553
1	F	0.48	0/1825	0.71	0/2498
1	G	0.44	0/1836	0.68	0/2515
1	H	0.45	0/1837	0.67	0/2516
1	I	0.51	0/1818	0.73	0/2488
1	J	0.50	1/1781 (0.1%)	0.73	0/2436
1	K	0.54	0/1811	0.74	0/2478
1	L	0.52	0/1837	0.73	0/2516
All	All	0.49	1/21817 (0.0%)	0.71	0/29865

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	77	CYS	CB-SG	-5.36	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1715	0	1689	74	0
1	B	1749	0	1733	77	0
1	C	1749	0	1732	91	0
1	D	1772	0	1755	78	0
1	E	1807	0	1781	61	0
1	F	1770	0	1751	68	0
1	G	1779	0	1762	91	0
1	H	1780	0	1757	126	0
1	I	1763	0	1744	51	0
1	J	1726	0	1703	47	0
1	K	1756	0	1739	58	0
1	L	1780	0	1759	54	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	2	0
2	I	10	0	0	0	0
2	J	15	0	0	2	0
2	K	10	0	0	1	0
2	L	10	0	0	0	0
3	A	10	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	1	0
3	D	3	0	0	0	0
3	E	8	0	0	0	0
3	F	9	0	0	0	0
3	G	3	0	0	0	0
3	H	4	0	0	0	0
3	I	12	0	0	0	0
3	J	7	0	0	0	0
3	K	12	0	0	1	0
3	L	12	0	0	0	0
All	All	21357	0	20905	742	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 18.

All (742) 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:231:LEU:H	1:B:177:GLN:NE2	1.49	1.09
1:I:60:LEU:HD13	1:I:60:LEU:H	1.16	1.05
1:E:1:MET:HE3	1:E:89:ASP:HB2	1.34	1.05
1:G:177:GLN:NE2	1:H:231:LEU:H	1.54	1.03
1:B:191:ASP:HB2	1:B:192:PRO:HD2	1.45	0.98
1:B:131:LEU:HG	1:B:132:ASN:H	1.21	0.98
1:F:195:ARG:HH22	1:H:48:ALA:HB3	1.29	0.97
1:E:75:ALA:HB1	1:E:116:GLN:HE21	1.31	0.95
1:G:177:GLN:HE22	1:H:231:LEU:H	1.15	0.94
1:G:231:LEU:H	1:H:177:GLN:NE2	1.64	0.94
1:G:58:SER:HB2	1:G:59:PRO:HD2	1.47	0.94
1:E:47:ILE:HD12	1:G:195:ARG:HH12	1.34	0.93
1:G:191:ASP:HB2	1:G:192:PRO:HD2	1.49	0.93
1:G:176:ARG:HB2	1:H:232:THR:HG21	1.52	0.92
1:J:100:ASN:H	1:J:164:ASN:HD21	1.18	0.91
1:A:1:MET:HB2	1:A:89:ASP:OD1	1.70	0.91
1:H:60:LEU:HD12	1:H:65:PHE:HZ	1.38	0.89
1:G:118:TYR:HD1	1:G:160:LEU:HB2	1.38	0.89
1:B:60:LEU:HD13	1:B:60:LEU:H	1.38	0.88
1:E:231:LEU:H	1:F:177:GLN:NE2	1.71	0.86
1:G:71:ARG:HH21	1:G:71:ARG:HG3	1.41	0.86
1:L:191:ASP:HB2	1:L:192:PRO:HD2	1.58	0.85
1:A:231:LEU:H	1:B:177:GLN:HE22	1.24	0.84
1:E:191:ASP:HB2	1:E:192:PRO:HD2	1.59	0.84
1:F:100:ASN:H	1:F:164:ASN:HD21	1.25	0.84
1:D:60:LEU:HD13	1:D:60:LEU:H	1.43	0.84
1:H:176:ARG:HG2	1:H:211:GLY:O	1.78	0.84
1:G:118:TYR:CD1	1:G:160:LEU:HB2	2.13	0.83
1:H:1:MET:HG3	1:H:89:ASP:HB2	1.60	0.83
1:H:60:LEU:HD12	1:H:65:PHE:CZ	2.14	0.83
1:J:205:LEU:O	1:J:206:LYS:HB3	1.78	0.83
1:D:45:ILE:HG23	1:D:47:ILE:HD13	1.62	0.81
1:K:191:ASP:HB2	1:K:192:PRO:HD2	1.62	0.81
1:F:131:LEU:HD11	1:F:136:PRO:HD3	1.62	0.81
1:G:231:LEU:H	1:H:177:GLN:HE22	1.25	0.81
1:B:47:ILE:HD12	1:D:195:ARG:NH1	1.97	0.80
1:D:45:ILE:HG23	1:D:47:ILE:CD1	2.12	0.79
1:E:100:ASN:H	1:E:164:ASN:HD21	1.31	0.78
1:C:100:ASN:H	1:C:164:ASN:HD21	1.32	0.77
1:F:47:ILE:HB	1:H:195:ARG:HH22	1.49	0.77
1:K:193:MET:HG3	1:K:195:ARG:HH21	1.51	0.76
1:K:193:MET:HG3	1:K:195:ARG:NH2	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE2	1:B:2:ARG:N	2.01	0.75
1:A:213:ASP:O	1:A:217:VAL:HG13	1.87	0.75
1:I:60:LEU:H	1:I:60:LEU:CD1	1.94	0.74
1:A:155:LEU:HD11	1:A:174:TRP:HH2	1.53	0.74
1:A:155:LEU:HD11	1:A:174:TRP:CH2	2.22	0.74
1:E:75:ALA:HB1	1:E:116:GLN:NE2	2.01	0.74
1:H:155:LEU:HD11	1:H:174:TRP:HH2	1.50	0.74
1:A:142:ARG:HB3	1:A:143:PRO:HD3	1.70	0.74
1:E:47:ILE:HB	1:G:195:ARG:CZ	2.17	0.73
1:E:1:MET:CE	1:E:89:ASP:HB2	2.16	0.73
1:A:108:SER:HB3	1:A:111:VAL:HB	1.70	0.73
1:H:131:LEU:HG	1:H:132:ASN:H	1.53	0.73
1:C:230:ASP:OD2	1:C:232:THR:HB	1.89	0.73
1:A:228:ARG:HD2	1:B:232:THR:O	1.88	0.73
1:A:69:ARG:HH12	1:A:71:ARG:HH11	1.37	0.73
1:B:200:PHE:CE2	1:B:202:PRO:HD3	2.24	0.72
1:C:231:LEU:H	1:D:177:GLN:NE2	1.87	0.72
1:C:48:ALA:HA	1:D:201:ALA:HB2	1.71	0.72
1:E:231:LEU:H	1:F:177:GLN:HE22	1.37	0.72
1:E:135:VAL:HG12	1:E:136:PRO:HD2	1.69	0.72
1:H:1:MET:HG3	1:H:89:ASP:CB	2.19	0.72
1:B:47:ILE:HB	1:D:195:ARG:NH1	2.04	0.72
1:G:177:GLN:NE2	1:H:231:LEU:N	2.36	0.71
1:H:191:ASP:HB2	1:H:192:PRO:HD2	1.72	0.71
1:G:231:LEU:O	1:H:228:ARG:HG2	1.90	0.71
1:A:180:ARG:HG2	1:A:206:LYS:HE2	1.70	0.71
1:J:56:HIS:HD2	1:J:69:ARG:HD3	1.54	0.71
1:D:191:ASP:HB2	1:D:192:PRO:HD2	1.73	0.71
1:A:231:LEU:N	1:B:177:GLN:NE2	2.33	0.71
1:B:56:HIS:HD2	1:B:69:ARG:HD3	1.56	0.71
1:K:231:LEU:H	1:L:177:GLN:NE2	1.89	0.70
1:C:30:PHE:HB3	1:C:85:PHE:CD1	2.26	0.70
1:K:200:PHE:CE1	1:K:202:PRO:HD3	2.25	0.70
1:L:144:TRP:CD1	1:L:169:PRO:HB2	2.26	0.70
1:I:100:ASN:H	1:I:164:ASN:HD21	1.40	0.69
1:A:49:HIS:CD2	1:A:49:HIS:H	2.10	0.69
1:B:47:ILE:HD12	1:D:195:ARG:HH12	1.58	0.69
1:B:195:ARG:NH1	1:D:47:ILE:HG22	2.08	0.69
1:I:200:PHE:CE2	1:I:202:PRO:HD3	2.28	0.69
1:A:1:MET:HG3	1:A:89:ASP:HB2	1.75	0.68
1:H:145:LEU:O	1:H:149:LEU:HG	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:LEU:HD12	1:D:123:SER:O	1.93	0.68
1:E:228:ARG:HD3	1:E:230:ASP:O	1.94	0.68
1:I:57:PRO:HG3	1:K:135:VAL:HG21	1.76	0.68
1:E:228:ARG:NH1	1:F:234:GLU:OE1	2.26	0.68
1:K:144:TRP:CE2	1:K:169:PRO:HB2	2.27	0.68
1:F:108:SER:HB3	1:F:111:VAL:HB	1.74	0.68
1:B:100:ASN:H	1:B:164:ASN:HD21	1.42	0.68
1:B:155:LEU:HD11	1:B:174:TRP:HH2	1.58	0.67
1:A:193:MET:HG2	1:D:203:ARG:CZ	2.24	0.67
1:D:121:GLY:O	1:D:122:LEU:HD23	1.93	0.67
1:H:46:THR:HG22	1:H:46:THR:O	1.94	0.67
1:E:47:ILE:HD12	1:G:195:ARG:NH1	2.08	0.67
1:A:231:LEU:N	1:B:177:GLN:HE22	1.92	0.66
1:G:142:ARG:HB3	1:G:143:PRO:HD3	1.77	0.66
1:F:191:ASP:OD2	1:F:193:MET:HB2	1.95	0.66
1:C:144:TRP:CD1	1:C:169:PRO:HB2	2.30	0.66
1:J:233:ASP:OD1	1:J:236:ARG:HG2	1.95	0.66
1:C:83:HIS:CD2	1:D:186:VAL:HB	2.31	0.66
1:G:144:TRP:CE2	1:G:169:PRO:HB2	2.31	0.66
1:A:231:LEU:H	1:B:177:GLN:HE21	1.42	0.66
1:D:121:GLY:C	1:D:122:LEU:HD23	2.17	0.66
1:I:60:LEU:HD13	1:I:60:LEU:N	2.00	0.65
1:A:228:ARG:NH1	1:A:230:ASP:O	2.30	0.65
1:A:52:ARG:NH1	1:B:197:PHE:HB3	2.10	0.65
1:B:47:ILE:HB	1:D:195:ARG:HH12	1.61	0.65
1:I:56:HIS:HD2	1:I:69:ARG:HD3	1.61	0.65
1:G:176:ARG:HH12	1:H:234:GLU:CG	2.09	0.65
1:C:129:VAL:HG23	1:C:130:PRO:HD2	1.78	0.65
1:A:158:PRO:HD3	1:I:143:PRO:HG3	1.78	0.65
1:G:176:ARG:CB	1:H:232:THR:HG21	2.24	0.64
1:H:91:VAL:HG23	1:H:122:LEU:HD12	1.78	0.64
1:G:2:ARG:HD3	1:G:87:PRO:O	1.97	0.64
1:F:130:PRO:O	1:F:131:LEU:HD12	1.98	0.64
1:F:47:ILE:HG12	1:H:195:ARG:HH12	1.63	0.64
1:C:228:ARG:NH2	1:D:228:ARG:NH1	2.44	0.64
1:H:190:GLU:HA	1:H:195:ARG:O	1.97	0.64
1:H:118:TYR:CD1	1:H:160:LEU:HB2	2.33	0.64
1:H:11:ILE:HG13	1:H:11:ILE:O	1.97	0.64
1:E:78:VAL:O	1:E:82:LEU:HG	1.98	0.64
1:B:176:ARG:HG2	1:B:211:GLY:O	1.96	0.64
1:L:146:LEU:O	1:L:150:GLU:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:ILE:HB	1:G:195:ARG:NH1	2.13	0.63
1:I:142:ARG:HB3	1:I:143:PRO:HD3	1.78	0.63
1:C:146:LEU:O	1:C:150:GLU:HG3	1.97	0.63
1:D:162:ASN:HB2	1:D:227:LEU:HD11	1.80	0.63
1:G:191:ASP:OD2	1:G:195:ARG:HB2	1.99	0.63
1:H:210:GLU:HG2	1:H:215:TRP:CE2	2.33	0.63
1:A:191:ASP:HB2	1:A:192:PRO:HD2	1.79	0.63
1:I:47:ILE:HG22	1:K:195:ARG:NH1	2.12	0.63
1:I:54:TYR:HE2	1:I:71:ARG:HD2	1.64	0.63
1:L:121:GLY:C	1:L:122:LEU:HD23	2.19	0.63
1:B:130:PRO:HG2	1:B:167:LEU:HG	1.79	0.63
1:A:115:LYS:HE2	1:B:106:TRP:CD2	2.34	0.63
1:I:88:VAL:HG12	1:I:122:LEU:HD13	1.81	0.62
1:C:191:ASP:HB2	1:C:192:PRO:HD2	1.81	0.62
1:H:155:LEU:HD11	1:H:174:TRP:CH2	2.33	0.62
1:L:76:ASP:O	1:L:80:LEU:HD13	1.99	0.62
1:D:183:GLU:HB3	1:D:205:LEU:HD21	1.80	0.62
1:F:181:ALA:H	1:F:206:LYS:HZ2	1.48	0.62
1:H:168:ARG:HH21	1:H:168:ARG:HG3	1.62	0.62
1:H:173:LEU:HD12	1:H:221:PHE:CD2	2.34	0.62
1:I:1:MET:CE	1:I:89:ASP:HB2	2.29	0.62
1:C:176:ARG:NH2	1:C:176:ARG:HB3	2.15	0.62
1:F:207:GLU:HA	1:F:207:GLU:OE1	2.00	0.62
1:A:198:TYR:CG	1:B:80:LEU:HD11	2.35	0.61
1:H:10:GLY:HA2	1:H:34:PRO:O	2.00	0.61
1:K:108:SER:HB3	1:K:111:VAL:HB	1.82	0.61
1:C:231:LEU:H	1:D:177:GLN:HE22	1.48	0.61
1:I:191:ASP:HB2	1:I:192:PRO:HD2	1.82	0.61
1:A:26:PHE:HE2	1:A:150:GLU:HG3	1.65	0.61
1:C:7:ASN:ND2	1:C:9:ASP:HB2	2.15	0.61
1:K:46:THR:HG22	1:L:202:PRO:HG2	1.82	0.61
1:C:168:ARG:HG3	1:C:168:ARG:HH21	1.65	0.61
1:F:171:GLY:HA3	1:F:221:PHE:HD1	1.65	0.61
1:K:21:GLU:O	1:K:24:SER:OG	2.18	0.61
1:A:78:VAL:O	1:A:82:LEU:HG	2.00	0.61
1:E:154:ARG:HB3	1:E:154:ARG:HH21	1.64	0.61
1:C:231:LEU:O	1:D:228:ARG:HG2	2.00	0.61
1:H:144:TRP:CD1	1:H:169:PRO:HB2	2.36	0.61
1:I:131:LEU:HG	1:I:132:ASN:H	1.66	0.60
1:I:233:ASP:OD2	1:I:236:ARG:NH2	2.32	0.60
1:K:100:ASN:H	1:K:164:ASN:HD21	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:237:LEU:C	1:I:237:LEU:HD23	2.22	0.60
1:G:58:SER:CB	1:G:59:PRO:HD2	2.26	0.60
1:B:131:LEU:HG	1:B:132:ASN:N	2.04	0.60
1:C:52:ARG:NH1	1:D:197:PHE:HB3	2.16	0.60
1:L:115:LYS:HG3	1:L:229:LEU:HD21	1.83	0.60
1:G:71:ARG:NH2	1:G:71:ARG:HG3	2.13	0.60
1:H:1:MET:HE3	1:H:3:ILE:HD11	1.84	0.60
1:F:131:LEU:O	1:F:132:ASN:HB2	2.02	0.60
1:G:175:THR:HG21	1:G:213:ASP:HA	1.84	0.60
1:J:75:ALA:HB1	1:J:116:GLN:HE21	1.65	0.59
1:C:48:ALA:CA	1:D:201:ALA:HB2	2.31	0.59
1:A:180:ARG:HG2	1:A:206:LYS:CE	2.31	0.59
1:G:155:LEU:HD11	1:G:174:TRP:CH2	2.37	0.59
1:C:181:ALA:HB3	1:C:205:LEU:HD22	1.83	0.59
1:G:173:LEU:HD12	1:G:221:PHE:CD2	2.37	0.59
1:A:49:HIS:HD2	1:A:49:HIS:H	1.48	0.59
1:F:183:GLU:OE1	1:F:203:ARG:NH1	2.33	0.59
1:J:142:ARG:HG2	1:J:142:ARG:HH11	1.66	0.59
1:H:213:ASP:OD2	1:H:214:ARG:N	2.35	0.59
1:G:86:GLY:HA2	1:G:88:VAL:HG23	1.84	0.59
1:B:144:TRP:CD1	1:B:169:PRO:HB2	2.37	0.59
1:H:35:ASP:HB3	1:H:69:ARG:HB2	1.84	0.59
1:C:11:ILE:O	1:C:11:ILE:HG13	2.02	0.59
1:J:185:VAL:HB	1:J:201:ALA:O	2.02	0.59
1:F:60:LEU:HD12	1:F:60:LEU:N	2.17	0.59
1:L:100:ASN:H	1:L:164:ASN:HD21	1.50	0.59
1:G:213:ASP:OD2	1:G:214:ARG:N	2.36	0.58
1:A:210:GLU:HA	1:A:215:TRP:CD2	2.38	0.58
1:H:147:ARG:O	1:H:147:ARG:HD3	2.03	0.58
1:E:197:PHE:HE1	1:E:199:TRP:CD1	2.21	0.58
1:G:134:GLU:CD	1:G:134:GLU:H	2.06	0.58
1:D:74:PRO:O	1:D:77:CYS:HB2	2.03	0.58
1:K:19:LEU:HB2	1:K:95:VAL:HG23	1.85	0.58
1:C:165:LEU:HD12	1:C:165:LEU:N	2.19	0.58
1:K:47:ILE:HD13	1:K:47:ILE:H	1.68	0.58
1:I:180:ARG:HG2	1:I:206:LYS:HE2	1.86	0.58
1:B:131:LEU:CG	1:B:132:ASN:H	2.01	0.58
1:L:142:ARG:HB3	1:L:143:PRO:HD3	1.86	0.58
1:C:1:MET:CE	1:C:153:LEU:HD22	2.34	0.58
1:G:177:GLN:HE22	1:H:231:LEU:N	1.96	0.57
1:G:231:LEU:HB2	1:H:177:GLN:NE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:THR:HG23	1:H:37:GLU:OE1	2.03	0.57
1:G:176:ARG:HH12	1:H:234:GLU:HG3	1.69	0.57
1:A:193:MET:HG2	1:D:203:ARG:NH1	2.19	0.57
1:E:73:THR:O	1:E:76:ASP:HB2	2.03	0.57
1:K:11:ILE:HG13	1:K:11:ILE:O	2.03	0.57
1:G:86:GLY:HA2	1:G:87:PRO:C	2.23	0.57
1:H:17:TRP:HZ3	1:H:65:PHE:HE2	1.50	0.57
1:H:140:GLY:O	1:H:143:PRO:HD2	2.04	0.57
1:F:47:ILE:C	1:F:47:ILE:HD12	2.26	0.57
1:G:155:LEU:HD11	1:G:174:TRP:HH2	1.70	0.57
1:I:228:ARG:NH1	1:I:230:ASP:O	2.37	0.57
1:K:142:ARG:O	1:K:146:LEU:HG	2.04	0.57
1:C:172:PHE:O	1:C:173:LEU:HD12	2.05	0.56
1:C:45:ILE:O	1:C:45:ILE:HD12	2.05	0.56
1:J:195:ARG:HG2	1:J:195:ARG:HH11	1.70	0.56
1:C:234:GLU:N	1:C:234:GLU:OE1	2.33	0.56
1:A:48:ALA:HB3	1:C:195:ARG:HH21	1.71	0.56
1:J:209:GLU:O	1:J:215:TRP:HB2	2.06	0.56
1:I:130:PRO:HD2	1:I:165:LEU:O	2.04	0.56
1:L:123:SER:OG	1:L:158:PRO:HA	2.06	0.56
1:G:131:LEU:HD22	1:G:132:ASN:N	2.21	0.56
1:G:177:GLN:OE1	1:H:231:LEU:HD12	2.06	0.56
1:H:47:ILE:HG13	1:H:47:ILE:O	2.06	0.56
1:G:56:HIS:HD2	1:G:69:ARG:HD3	1.71	0.56
1:C:131:LEU:HG	1:C:132:ASN:H	1.71	0.56
1:C:154:ARG:HH21	1:C:154:ARG:CB	2.19	0.56
1:F:155:LEU:HD11	1:F:174:TRP:HH2	1.70	0.56
1:C:230:ASP:HA	1:D:177:GLN:NE2	2.20	0.56
1:D:131:LEU:HD21	1:D:136:PRO:HD3	1.88	0.56
1:J:71:ARG:HD2	1:L:132:ASN:HD21	1.71	0.56
1:F:47:ILE:CD1	1:H:195:ARG:HH12	2.19	0.56
1:C:176:ARG:O	1:C:212:THR:HA	2.06	0.56
1:C:163:VAL:HA	1:C:223:SER:O	2.06	0.55
1:K:8:ASP:OD2	1:K:8:ASP:C	2.45	0.55
1:G:231:LEU:N	1:H:177:GLN:HE22	1.99	0.55
1:D:100:ASN:H	1:D:164:ASN:HD21	1.54	0.55
1:H:183:GLU:OE2	1:H:203:ARG:NH1	2.39	0.55
1:L:210:GLU:HG2	1:L:215:TRP:NE1	2.21	0.55
1:G:206:LYS:O	1:G:206:LYS:HD2	2.06	0.55
1:D:142:ARG:O	1:D:146:LEU:HG	2.07	0.55
1:H:1:MET:CE	1:H:3:ILE:HD11	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:ILE:HG22	1:K:195:ARG:HH12	1.71	0.55
1:H:172:PHE:O	1:H:173:LEU:HB2	2.07	0.55
1:B:24:SER:HA	1:B:29:VAL:HG23	1.89	0.55
1:B:191:ASP:HB2	1:B:192:PRO:CD	2.28	0.55
1:D:203:ARG:HD2	1:E:242:ALA:HB1	1.89	0.55
1:E:200:PHE:CE2	1:E:202:PRO:HD3	2.41	0.55
1:H:131:LEU:HD12	1:H:134:GLU:O	2.07	0.55
1:F:171:GLY:HA3	1:F:221:PHE:CD1	2.41	0.55
1:H:200:PHE:CE2	1:H:202:PRO:HD3	2.41	0.54
1:B:47:ILE:CD1	1:D:195:ARG:HH12	2.20	0.54
1:F:47:ILE:HB	1:H:195:ARG:NH2	2.19	0.54
1:H:173:LEU:HD12	1:H:221:PHE:HD2	1.71	0.54
1:J:191:ASP:HB2	1:J:192:PRO:HD2	1.89	0.54
1:A:186:VAL:HA	1:A:199:TRP:O	2.06	0.54
1:G:191:ASP:HB2	1:G:192:PRO:CD	2.32	0.54
1:L:237:LEU:O	1:L:238:GLN:C	2.45	0.54
1:L:206:LYS:HE3	1:L:209:GLU:OE2	2.07	0.54
1:L:26:PHE:HE2	1:L:150:GLU:HG2	1.73	0.54
1:E:48:ALA:HB3	1:G:195:ARG:HH21	1.73	0.54
1:B:47:ILE:CG1	1:D:195:ARG:HH12	2.21	0.54
1:G:30:PHE:HB3	1:G:85:PHE:CD1	2.42	0.54
1:D:235:THR:HG22	1:D:236:ARG:N	2.22	0.54
1:C:234:GLU:H	1:C:234:GLU:CD	2.06	0.54
1:K:7:ASN:C	1:K:7:ASN:OD1	2.46	0.54
1:C:156:GLU:O	1:C:156:GLU:HG3	2.07	0.54
1:F:47:ILE:CG1	1:H:195:ARG:HH12	2.19	0.54
1:K:193:MET:CG	1:K:195:ARG:HH21	2.20	0.54
1:C:52:ARG:HH22	1:D:195:ARG:NH2	2.06	0.53
1:G:85:PHE:O	1:G:86:GLY:O	2.26	0.53
1:J:102:GLY:HA3	2:J:1202:PO4:O2	2.07	0.53
2:C:501:PO4:O2	3:C:503:HOH:O	2.19	0.53
1:E:197:PHE:HB3	1:F:52:ARG:NH1	2.23	0.53
1:B:78:VAL:O	1:B:82:LEU:HG	2.09	0.53
1:B:147:ARG:O	1:B:147:ARG:HD3	2.07	0.53
1:G:155:LEU:HB3	1:H:236:ARG:NH1	2.23	0.53
1:K:2:ARG:HD3	1:K:87:PRO:O	2.09	0.53
1:H:29:VAL:HG12	1:H:30:PHE:N	2.23	0.53
1:G:231:LEU:N	1:H:177:GLN:NE2	2.47	0.53
1:C:168:ARG:NH2	1:C:168:ARG:HG3	2.23	0.53
1:B:1:MET:HG2	1:B:26:PHE:O	2.09	0.53
1:J:6:THR:OG1	1:J:7:ASN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:TRP:CD2	1:H:115:LYS:HE2	2.43	0.53
1:D:75:ALA:HB1	1:D:116:GLN:HE21	1.74	0.53
1:H:123:SER:HB3	1:H:159:PHE:CE2	2.43	0.53
1:A:48:ALA:HB3	1:C:195:ARG:NH2	2.24	0.53
1:I:177:GLN:NE2	1:J:231:LEU:H	2.07	0.53
1:K:230:ASP:HA	1:L:177:GLN:NE2	2.24	0.52
1:J:90:LEU:HD21	1:J:92:LEU:HD21	1.92	0.52
1:C:65:PHE:N	1:C:65:PHE:CD1	2.77	0.52
1:J:56:HIS:CD2	1:J:69:ARG:HD3	2.42	0.52
1:C:152:LEU:O	1:C:155:LEU:HB2	2.09	0.52
1:A:56:HIS:O	1:A:67:ALA:HB3	2.09	0.52
1:H:47:ILE:O	1:H:48:ALA:C	2.46	0.52
1:C:181:ALA:CB	1:C:205:LEU:HD22	2.40	0.52
1:F:172:PHE:O	1:F:173:LEU:HD23	2.09	0.52
1:J:90:LEU:HD12	1:J:123:SER:O	2.09	0.52
1:K:6:THR:O	1:K:93:SER:HA	2.09	0.52
1:K:228:ARG:NH1	1:L:228:ARG:CZ	2.73	0.52
1:D:8:ASP:C	1:D:8:ASP:OD2	2.45	0.52
1:I:60:LEU:O	1:I:62:ALA:N	2.42	0.52
1:B:195:ARG:HH12	1:D:47:ILE:HG22	1.74	0.52
1:E:185:VAL:HB	1:E:201:ALA:O	2.09	0.52
1:A:173:LEU:HD12	1:A:221:PHE:HD2	1.75	0.52
1:G:45:ILE:HG22	1:G:49:HIS:HD2	1.74	0.52
1:B:206:LYS:HG2	1:B:207:GLU:O	2.09	0.52
1:B:155:LEU:HD11	1:B:174:TRP:CH2	2.43	0.52
1:G:86:GLY:HA2	1:G:87:PRO:O	2.10	0.52
1:G:172:PHE:CD2	1:G:173:LEU:N	2.78	0.52
1:A:80:LEU:HD11	1:B:198:TYR:CD1	2.44	0.52
1:B:213:ASP:OD2	1:B:214:ARG:N	2.41	0.52
1:D:123:SER:OG	1:D:158:PRO:HA	2.10	0.52
1:E:200:PHE:HD1	1:F:76:ASP:OD1	1.92	0.52
1:F:47:ILE:O	1:F:49:HIS:ND1	2.43	0.51
1:G:100:ASN:H	1:G:164:ASN:HD21	1.57	0.51
1:H:137:ASP:OD2	1:H:139:ALA:HB3	2.10	0.51
1:F:181:ALA:H	1:F:206:LYS:NZ	2.08	0.51
1:B:132:ASN:HD22	1:D:71:ARG:HD2	1.75	0.51
1:H:168:ARG:NH2	1:H:168:ARG:HG3	2.26	0.51
1:L:35:ASP:OD2	1:L:71:ARG:NH1	2.43	0.51
1:I:19:LEU:HB2	1:I:95:VAL:HG23	1.90	0.51
1:H:185:VAL:HB	1:H:201:ALA:O	2.10	0.51
1:B:47:ILE:CB	1:D:195:ARG:HH12	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:ARG:NH1	1:J:142:ARG:HG2	2.26	0.51
1:C:141:LEU:C	1:C:143:PRO:HD2	2.31	0.51
1:E:147:ARG:NH1	1:E:151:THR:OG1	2.44	0.51
1:D:85:PHE:O	1:D:86:GLY:C	2.49	0.51
1:G:58:SER:HB2	1:G:59:PRO:CD	2.31	0.51
1:H:210:GLU:HG2	1:H:215:TRP:CZ2	2.46	0.51
1:C:86:GLY:HA2	1:C:87:PRO:O	2.11	0.51
1:D:130:PRO:HD2	1:D:165:LEU:O	2.11	0.51
1:G:178:SER:HB2	1:G:212:THR:HB	1.93	0.51
1:C:228:ARG:NH2	1:D:228:ARG:CZ	2.74	0.51
1:G:234:GLU:OE1	1:H:176:ARG:NH2	2.42	0.50
1:C:172:PHE:CD2	1:C:173:LEU:N	2.79	0.50
1:A:48:ALA:HB2	1:C:193:MET:HE3	1.93	0.50
1:J:184:GLY:O	1:J:186:VAL:HG23	2.11	0.50
1:H:165:LEU:N	1:H:165:LEU:HD12	2.25	0.50
1:H:35:ASP:OD1	1:H:36:THR:HG23	2.10	0.50
1:G:182:TYR:CE2	1:G:204:PRO:HD3	2.46	0.50
1:D:203:ARG:HD2	1:E:242:ALA:CB	2.41	0.50
1:I:52:ARG:HB2	1:I:71:ARG:HD3	1.93	0.50
1:E:154:ARG:HH21	1:E:154:ARG:CB	2.23	0.50
1:H:49:HIS:CE1	1:H:76:ASP:OD2	2.64	0.50
1:L:26:PHE:CE2	1:L:150:GLU:HG2	2.46	0.50
1:H:100:ASN:H	1:H:164:ASN:HD21	1.58	0.50
1:B:60:LEU:H	1:B:60:LEU:CD1	2.16	0.50
1:D:45:ILE:HG23	1:D:47:ILE:HD11	1.90	0.50
1:D:19:LEU:HB2	1:D:95:VAL:HG23	1.94	0.50
1:E:210:GLU:HB2	1:E:215:TRP:CE2	2.46	0.50
1:C:52:ARG:NH2	1:D:195:ARG:NH2	2.60	0.50
1:F:47:ILE:HD13	1:H:195:ARG:NH2	2.27	0.50
1:K:200:PHE:CD1	1:K:202:PRO:HD3	2.45	0.50
1:F:35:ASP:OD2	1:F:69:ARG:NH2	2.45	0.50
1:K:75:ALA:HB1	1:K:116:GLN:HE21	1.76	0.50
1:I:56:HIS:CD2	1:I:69:ARG:HD3	2.45	0.50
1:L:26:PHE:CD2	1:L:153:LEU:HD12	2.47	0.50
1:A:200:PHE:HD1	1:B:76:ASP:OD1	1.95	0.50
1:I:78:VAL:O	1:I:82:LEU:HG	2.11	0.49
1:B:210:GLU:HA	1:B:215:TRP:CG	2.47	0.49
1:D:60:LEU:HD13	1:D:60:LEU:N	2.20	0.49
1:K:30:PHE:HB3	1:K:85:PHE:CD1	2.48	0.49
1:C:161:VAL:HG11	1:C:224:ALA:HB1	1.94	0.49
1:I:183:GLU:HB2	1:I:205:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ARG:HD3	1:B:87:PRO:O	2.13	0.49
1:G:56:HIS:CD2	1:G:69:ARG:HD3	2.48	0.49
1:G:165:LEU:N	1:G:165:LEU:HD12	2.27	0.49
1:A:228:ARG:NH1	1:B:228:ARG:HD3	2.27	0.49
1:F:191:ASP:O	1:F:193:MET:N	2.46	0.49
1:L:62:ALA:HB1	1:L:63:PRO:CD	2.42	0.49
1:H:172:PHE:CG	1:H:173:LEU:N	2.80	0.49
1:E:68:TYR:CZ	1:E:84:LEU:HD13	2.48	0.49
1:F:90:LEU:HD21	1:F:92:LEU:HD21	1.94	0.49
1:I:68:TYR:CE2	1:I:84:LEU:HD13	2.48	0.49
1:J:170:LYS:HE3	1:J:220:GLY:HA3	1.93	0.49
1:G:228:ARG:HG2	1:H:231:LEU:O	2.13	0.49
1:F:47:ILE:HD13	1:H:195:ARG:HH22	1.77	0.49
1:B:192:PRO:C	1:B:194:GLY:H	2.16	0.49
1:A:198:TYR:HE2	1:B:53:ALA:HB3	1.78	0.49
1:C:142:ARG:N	1:C:143:PRO:CD	2.75	0.49
1:H:49:HIS:HE1	1:H:76:ASP:OD2	1.95	0.49
1:B:138:PHE:HA	1:B:141:LEU:HB2	1.95	0.49
1:H:71:ARG:HG2	1:H:71:ARG:HH11	1.77	0.49
1:F:190:GLU:OE1	1:F:194:GLY:HA2	2.12	0.48
1:E:47:ILE:HB	1:G:195:ARG:NH2	2.28	0.48
1:I:110:THR:HG22	1:I:126:ALA:HB1	1.94	0.48
1:C:110:THR:HG22	1:C:126:ALA:HB1	1.96	0.48
1:G:177:GLN:HB3	1:H:230:ASP:OD2	2.13	0.48
1:H:175:THR:HG1	1:H:225:THR:HG1	1.60	0.48
1:H:106:TRP:CH2	1:H:231:LEU:HD22	2.48	0.48
1:A:173:LEU:HD12	1:A:221:PHE:CD2	2.49	0.48
1:C:106:TRP:CH2	1:C:231:LEU:HD22	2.48	0.48
1:C:178:SER:HB2	1:C:212:THR:HB	1.93	0.48
1:L:215:TRP:O	1:L:219:GLN:HG2	2.14	0.48
1:D:142:ARG:HB3	1:D:143:PRO:HD3	1.95	0.48
1:A:198:TYR:HB2	1:B:80:LEU:HD21	1.95	0.48
1:H:161:VAL:HG12	1:H:162:ASN:N	2.28	0.48
1:D:53:ALA:HB2	1:D:80:LEU:HD23	1.94	0.48
1:H:209:GLU:O	1:H:212:THR:HG23	2.13	0.48
1:C:30:PHE:HB3	1:C:85:PHE:CE1	2.48	0.48
1:H:172:PHE:O	1:H:173:LEU:CB	2.62	0.48
1:H:2:ARG:HB3	1:H:30:PHE:HE2	1.79	0.48
2:K:1301:PO4:O2	3:K:1310:HOH:O	2.20	0.48
1:E:131:LEU:O	1:E:132:ASN:HB2	2.14	0.48
1:L:118:TYR:CD1	1:L:160:LEU:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:TRP:CE2	1:H:115:LYS:HE2	2.49	0.48
1:H:141:LEU:HD21	1:H:167:LEU:O	2.13	0.48
1:H:187:ILE:HD12	1:H:187:ILE:N	2.28	0.48
1:C:167:LEU:O	1:C:169:PRO:HD3	2.14	0.48
1:E:210:GLU:HA	1:E:215:TRP:CG	2.49	0.48
1:L:176:ARG:HG2	1:L:211:GLY:O	2.14	0.48
1:F:140:GLY:O	1:F:143:PRO:HD2	2.14	0.48
1:K:98:GLY:O	1:K:128:SER:HB3	2.13	0.48
1:F:125:ALA:HA	1:F:161:VAL:O	2.12	0.48
1:A:231:LEU:O	1:B:228:ARG:HG2	2.14	0.48
1:C:86:GLY:HA2	1:C:88:VAL:HG23	1.96	0.48
1:L:176:ARG:HB3	1:L:176:ARG:NH2	2.29	0.47
1:F:210:GLU:HA	1:F:215:TRP:CD2	2.50	0.47
1:B:200:PHE:CD2	1:B:202:PRO:HD3	2.48	0.47
1:D:210:GLU:HG2	1:D:215:TRP:CE2	2.48	0.47
1:G:177:GLN:N	1:H:232:THR:OG1	2.36	0.47
1:B:162:ASN:HB2	1:B:227:LEU:HD11	1.96	0.47
1:G:144:TRP:NE1	1:G:169:PRO:HB2	2.29	0.47
1:I:115:LYS:HE2	1:J:106:TRP:CD2	2.49	0.47
1:J:206:LYS:HG2	1:J:207:GLU:O	2.14	0.47
1:A:69:ARG:HH22	1:A:71:ARG:HG2	1.80	0.47
1:H:145:LEU:HD23	1:H:165:LEU:HD21	1.97	0.47
1:L:122:LEU:N	1:L:122:LEU:HD23	2.29	0.47
1:I:191:ASP:OD2	1:I:191:ASP:C	2.53	0.47
1:L:131:LEU:CG	1:L:132:ASN:H	2.28	0.47
1:L:129:VAL:HG23	1:L:130:PRO:HD2	1.96	0.47
1:G:17:TRP:CE3	1:G:59:PRO:HD3	2.50	0.47
1:C:48:ALA:CB	1:D:201:ALA:HB2	2.45	0.47
1:B:69:ARG:NH1	1:D:131:LEU:HD12	2.30	0.47
1:A:52:ARG:HH11	1:B:197:PHE:HB3	1.80	0.47
1:E:197:PHE:HB3	1:F:52:ARG:HH11	1.79	0.47
1:I:69:ARG:HH12	1:K:132:ASN:HA	1.79	0.47
1:H:102:GLY:HA3	2:H:1002:PO4:O2	2.15	0.47
1:B:118:TYR:CD1	1:B:160:LEU:HB2	2.49	0.47
1:A:163:VAL:HA	1:A:223:SER:O	2.14	0.47
1:C:235:THR:O	1:C:236:ARG:HG2	2.14	0.47
1:A:101:LEU:O	1:A:104:GLU:HB2	2.14	0.47
1:H:186:VAL:HA	1:H:199:TRP:O	2.15	0.47
1:A:69:ARG:HH12	1:A:71:ARG:NH1	2.08	0.47
1:G:6:THR:O	1:G:93:SER:HA	2.15	0.47
1:A:17:TRP:CE3	1:A:59:PRO:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2:ARG:NH1	1:K:87:PRO:O	2.44	0.46
1:H:191:ASP:OD2	1:H:195:ARG:HB2	2.15	0.46
1:C:86:GLY:HA2	1:C:87:PRO:C	2.36	0.46
1:A:200:PHE:CZ	1:B:79:ALA:HB2	2.50	0.46
1:G:231:LEU:HB2	1:H:177:GLN:HE22	1.78	0.46
1:F:47:ILE:O	1:F:48:ALA:C	2.51	0.46
1:D:131:LEU:CD2	1:D:136:PRO:HD3	2.45	0.46
1:K:231:LEU:H	1:L:177:GLN:HE22	1.61	0.46
1:J:169:PRO:HB3	1:J:222:VAL:HG23	1.96	0.46
1:K:76:ASP:OD2	1:L:200:PHE:HD1	1.99	0.46
1:H:30:PHE:HB3	1:H:85:PHE:CE1	2.51	0.46
1:K:172:PHE:O	1:K:173:LEU:HG	2.14	0.46
1:D:170:LYS:HE3	1:D:219:GLN:O	2.15	0.46
1:B:30:PHE:CD1	1:B:85:PHE:CD2	3.04	0.46
1:C:83:HIS:CG	1:D:186:VAL:HB	2.50	0.46
1:B:197:PHE:HE1	1:B:199:TRP:CD1	2.33	0.46
1:K:175:THR:O	1:L:237:LEU:HD21	2.16	0.46
1:E:142:ARG:HB3	1:E:143:PRO:HD3	1.98	0.46
1:F:191:ASP:OD2	1:F:195:ARG:NH1	2.48	0.46
1:A:48:ALA:CB	1:C:195:ARG:NH2	2.78	0.46
1:C:123:SER:HB3	1:C:159:PHE:CE2	2.51	0.46
1:E:90:LEU:HD12	1:E:123:SER:O	2.15	0.46
1:C:5:VAL:HG22	1:C:92:LEU:HB2	1.97	0.46
1:F:6:THR:OG1	1:F:7:ASN:N	2.48	0.46
1:J:130:PRO:HD2	1:J:165:LEU:O	2.15	0.46
1:G:61:HIS:O	1:G:62:ALA:HB2	2.15	0.46
1:K:142:ARG:HB3	1:K:143:PRO:HD3	1.97	0.45
1:H:30:PHE:HB3	1:H:85:PHE:CZ	2.51	0.45
1:K:85:PHE:O	1:K:86:GLY:C	2.54	0.45
1:I:123:SER:OG	1:I:158:PRO:HA	2.16	0.45
1:H:19:LEU:HB2	1:H:95:VAL:HG23	1.97	0.45
1:L:75:ALA:HB1	1:L:116:GLN:HE21	1.79	0.45
1:L:228:ARG:HD3	1:L:230:ASP:O	2.16	0.45
1:L:148:THR:HG23	1:L:172:PHE:HE1	1.80	0.45
1:K:155:LEU:HD21	1:K:174:TRP:CZ2	2.51	0.45
1:L:178:SER:HB2	1:L:212:THR:HB	1.98	0.45
1:I:118:TYR:CD2	1:I:229:LEU:HD11	2.52	0.45
1:J:152:LEU:O	1:J:155:LEU:HB2	2.17	0.45
1:G:228:ARG:NH1	1:H:228:ARG:CZ	2.79	0.45
1:H:172:PHE:CD2	1:H:173:LEU:N	2.84	0.45
1:A:198:TYR:CD2	1:B:80:LEU:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:35:ASP:OD1	1:J:71:ARG:NH1	2.50	0.45
1:F:21:GLU:O	1:F:24:SER:OG	2.30	0.45
1:G:8:ASP:C	1:G:8:ASP:OD2	2.55	0.45
1:J:142:ARG:HB3	1:J:143:PRO:HD3	1.97	0.45
1:H:200:PHE:CD2	1:H:202:PRO:HD3	2.50	0.45
1:J:123:SER:HB3	1:J:159:PHE:CZ	2.52	0.45
1:C:231:LEU:CD2	1:D:231:LEU:HD21	2.47	0.45
1:B:73:THR:O	1:B:76:ASP:HB2	2.16	0.45
1:K:213:ASP:OD2	1:K:214:ARG:N	2.49	0.45
1:I:200:PHE:CD2	1:I:202:PRO:HD3	2.50	0.45
1:K:131:LEU:HG	1:K:132:ASN:H	1.82	0.45
1:F:180:ARG:HG2	1:F:206:LYS:HE2	1.99	0.45
1:C:35:ASP:HB2	1:C:71:ARG:HA	1.99	0.45
1:G:176:ARG:O	1:G:212:THR:HA	2.17	0.45
1:E:56:HIS:O	1:E:67:ALA:HB3	2.17	0.45
1:A:185:VAL:HB	1:A:201:ALA:O	2.17	0.45
1:I:35:ASP:OD1	1:I:71:ARG:NH1	2.50	0.45
1:J:95:VAL:CG2	1:J:129:VAL:HG13	2.47	0.45
1:E:172:PHE:C	1:E:172:PHE:CD2	2.90	0.45
1:A:26:PHE:CE2	1:A:150:GLU:HG3	2.49	0.44
1:K:170:LYS:HB3	1:K:170:LYS:HE2	1.75	0.44
1:J:2:ARG:HD3	1:J:87:PRO:O	2.18	0.44
1:J:163:VAL:HA	1:J:223:SER:O	2.18	0.44
1:I:4:LEU:HD12	1:I:30:PHE:O	2.17	0.44
1:D:96:ASN:HD22	1:D:100:ASN:ND2	2.16	0.44
1:H:161:VAL:HG11	1:H:224:ALA:HB1	1.99	0.44
1:B:132:ASN:ND2	1:D:71:ARG:HD2	2.32	0.44
1:E:191:ASP:HB2	1:E:192:PRO:CD	2.41	0.44
1:J:228:ARG:NH2	1:J:230:ASP:O	2.49	0.44
1:E:144:TRP:CD1	1:E:169:PRO:HB2	2.52	0.44
1:C:6:THR:O	1:C:93:SER:HA	2.18	0.44
1:K:106:TRP:CH2	1:K:231:LEU:HD13	2.52	0.44
1:G:134:GLU:N	1:G:134:GLU:CD	2.71	0.44
1:C:131:LEU:HG	1:C:132:ASN:N	2.33	0.44
1:H:146:LEU:O	1:H:150:GLU:HG3	2.18	0.44
1:I:185:VAL:HB	1:I:201:ALA:O	2.17	0.44
1:B:60:LEU:N	1:B:60:LEU:HD13	2.19	0.44
1:A:172:PHE:CD2	1:A:173:LEU:N	2.86	0.44
1:A:115:LYS:HE2	1:B:106:TRP:CE3	2.51	0.44
1:F:155:LEU:HD11	1:F:174:TRP:CH2	2.51	0.44
1:B:175:THR:O	1:B:225:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:203:ARG:O	1:J:203:ARG:HG3	2.18	0.44
1:B:165:LEU:HD12	1:B:165:LEU:N	2.33	0.44
1:C:84:LEU:HD21	1:D:198:TYR:OH	2.18	0.44
1:F:191:ASP:C	1:F:193:MET:H	2.21	0.44
1:K:78:VAL:O	1:K:82:LEU:HG	2.18	0.44
1:H:131:LEU:CG	1:H:132:ASN:H	2.21	0.44
1:H:134:GLU:CD	1:H:167:LEU:CD1	2.87	0.44
1:C:1:MET:HE3	1:C:153:LEU:HD22	1.99	0.44
1:C:81:GLY:O	1:C:85:PHE:HB2	2.18	0.44
1:D:101:LEU:HD22	1:D:213:ASP:HB2	2.00	0.44
1:K:101:LEU:O	1:K:104:GLU:HB2	2.18	0.44
1:H:8:ASP:OD1	2:H:1001:PO4:O2	2.35	0.44
1:E:183:GLU:O	1:E:183:GLU:HG3	2.18	0.44
1:F:7:ASN:OD1	1:F:7:ASN:C	2.57	0.43
1:B:75:ALA:HB1	1:B:116:GLN:NE2	2.33	0.43
1:E:191:ASP:CB	1:E:192:PRO:HD2	2.42	0.43
1:H:46:THR:O	1:H:46:THR:CG2	2.65	0.43
1:F:185:VAL:HB	1:F:201:ALA:O	2.18	0.43
1:A:234:GLU:C	1:A:236:ARG:H	2.20	0.43
1:A:141:LEU:HD21	1:A:167:LEU:O	2.18	0.43
1:C:230:ASP:OD1	1:D:177:GLN:HB3	2.18	0.43
1:E:154:ARG:CB	1:E:154:ARG:NH2	2.82	0.43
1:F:191:ASP:OD1	1:F:195:ARG:HB2	2.18	0.43
1:C:154:ARG:NH2	1:C:154:ARG:HB2	2.33	0.43
1:A:203:ARG:HH11	1:A:203:ARG:HG2	1.84	0.43
1:B:105:ILE:HG23	1:B:111:VAL:HG21	1.99	0.43
1:C:203:ARG:HH11	1:C:203:ARG:HG3	1.83	0.43
1:H:1:MET:HE1	1:H:26:PHE:O	2.17	0.43
1:B:1:MET:O	1:B:1:MET:HG3	2.19	0.43
1:L:131:LEU:HG	1:L:132:ASN:H	1.83	0.43
1:H:90:LEU:HD21	1:H:92:LEU:HD21	2.01	0.43
1:I:8:ASP:C	1:I:8:ASP:OD2	2.56	0.43
1:J:195:ARG:HG2	1:J:195:ARG:NH1	2.33	0.43
1:G:35:ASP:OD2	1:G:69:ARG:HD2	2.19	0.43
1:C:213:ASP:O	1:C:217:VAL:HG13	2.18	0.43
1:J:8:ASP:OD2	1:J:8:ASP:C	2.57	0.43
1:C:176:ARG:CZ	1:C:176:ARG:CB	2.96	0.43
1:A:48:ALA:CB	1:C:195:ARG:HH21	2.31	0.43
1:K:232:THR:HG22	1:K:233:ASP:N	2.34	0.43
1:G:181:ALA:HB3	1:G:205:LEU:HD22	2.00	0.43
1:I:60:LEU:O	1:I:62:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:HD13	1:B:80:LEU:HA	1.82	0.43
1:E:123:SER:OG	1:E:158:PRO:HA	2.19	0.43
1:F:228:ARG:NH2	1:F:230:ASP:O	2.48	0.43
1:E:118:TYR:CD2	1:E:229:LEU:HD11	2.54	0.43
1:D:47:ILE:N	1:D:47:ILE:HD13	2.34	0.43
1:C:231:LEU:HD21	1:D:231:LEU:HD21	2.00	0.43
1:A:177:GLN:HE22	1:B:231:LEU:HD12	1.84	0.43
1:I:166:PRO:HG2	1:I:169:PRO:HG3	2.01	0.43
1:L:11:ILE:O	1:L:11:ILE:HG13	2.19	0.43
1:A:54:TYR:HE2	1:A:71:ARG:HD2	1.83	0.43
1:A:24:SER:HB3	1:A:65:PHE:HE1	1.84	0.43
1:F:129:VAL:HG23	1:F:165:LEU:O	2.19	0.42
1:H:147:ARG:HD3	1:H:147:ARG:C	2.39	0.42
1:H:9:ASP:HA	1:H:37:GLU:OE2	2.18	0.42
1:C:70:VAL:O	1:C:72:GLY:N	2.50	0.42
1:I:210:GLU:HA	1:I:215:TRP:CD2	2.53	0.42
1:G:106:TRP:CD1	1:H:231:LEU:HD11	2.54	0.42
1:I:11:ILE:HD13	1:I:56:HIS:CG	2.54	0.42
1:K:163:VAL:HA	1:K:223:SER:O	2.19	0.42
1:F:118:TYR:CD2	1:F:229:LEU:HD11	2.54	0.42
1:H:74:PRO:O	1:H:77:CYS:HB2	2.18	0.42
1:H:110:THR:HG22	1:H:126:ALA:HB1	1.99	0.42
1:D:172:PHE:CD2	1:D:173:LEU:N	2.87	0.42
1:E:48:ALA:HA	1:F:200:PHE:O	2.19	0.42
1:B:129:VAL:HG23	1:B:130:PRO:HD2	2.01	0.42
1:J:142:ARG:O	1:J:146:LEU:HG	2.19	0.42
1:G:182:TYR:HE2	1:G:204:PRO:HD3	1.84	0.42
1:G:130:PRO:HD2	1:G:165:LEU:O	2.19	0.42
1:D:68:TYR:CZ	1:D:84:LEU:HD13	2.55	0.42
1:G:208:ALA:O	1:G:209:GLU:O	2.36	0.42
1:E:228:ARG:HG2	1:F:231:LEU:O	2.19	0.42
1:F:118:TYR:HD2	1:F:229:LEU:HD11	1.83	0.42
1:G:109:GLY:O	1:G:112:ALA:HB3	2.20	0.42
1:J:132:ASN:HA	1:J:132:ASN:HD22	1.57	0.42
1:B:209:GLU:O	1:B:212:THR:HG23	2.19	0.42
1:C:92:LEU:HD22	1:C:127:PHE:CE1	2.55	0.42
1:L:6:THR:O	1:L:93:SER:HA	2.18	0.42
1:H:176:ARG:NH2	1:H:176:ARG:HB3	2.35	0.42
1:C:177:GLN:OE1	1:D:231:LEU:N	2.39	0.42
1:G:30:PHE:HB3	1:G:85:PHE:CE1	2.54	0.42
1:C:176:ARG:HH21	1:C:176:ARG:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:142:ARG:N	1:H:143:PRO:CD	2.83	0.42
1:E:118:TYR:HD2	1:E:229:LEU:HD11	1.84	0.42
1:D:118:TYR:CD1	1:D:160:LEU:HB2	2.55	0.42
1:C:64:HIS:C	1:C:64:HIS:ND1	2.73	0.42
1:C:106:TRP:CZ2	1:C:231:LEU:HD22	2.55	0.42
1:K:131:LEU:HG	1:K:132:ASN:N	2.35	0.42
1:L:7:ASN:ND2	1:L:16:LEU:HB2	2.34	0.42
1:E:98:GLY:N	1:E:129:VAL:O	2.52	0.42
1:A:237:LEU:HD13	1:A:237:LEU:O	2.19	0.42
1:G:210:GLU:HG2	1:G:215:TRP:CE2	2.55	0.42
1:D:197:PHE:CD1	1:D:197:PHE:C	2.92	0.42
1:H:122:LEU:HD23	1:H:122:LEU:N	2.34	0.42
1:A:198:TYR:CB	1:B:80:LEU:HD21	2.49	0.42
1:F:53:ALA:HB2	1:F:80:LEU:CD2	2.50	0.42
1:E:48:ALA:O	1:G:195:ARG:NH2	2.53	0.42
1:G:71:ARG:NH2	1:G:71:ARG:CG	2.79	0.42
1:F:47:ILE:HD13	1:H:195:ARG:NH1	2.35	0.42
1:A:35:ASP:OD2	1:A:69:ARG:NH2	2.53	0.42
1:E:106:TRP:CD2	1:F:115:LYS:HE2	2.55	0.42
1:A:8:ASP:OD2	1:A:8:ASP:C	2.58	0.42
1:B:56:HIS:CD2	1:B:69:ARG:HD3	2.45	0.42
1:L:106:TRP:CZ3	1:L:231:LEU:HD13	2.54	0.42
1:C:192:PRO:C	1:C:194:GLY:H	2.24	0.42
1:H:29:VAL:CG1	1:H:30:PHE:N	2.83	0.42
1:K:172:PHE:CD2	1:K:173:LEU:N	2.88	0.42
1:C:92:LEU:HD22	1:C:127:PHE:HE1	1.84	0.42
1:A:183:GLU:CD	1:A:203:ARG:HH12	2.23	0.42
1:K:45:ILE:HD12	1:K:45:ILE:O	2.20	0.42
1:E:33:ALA:HA	1:E:34:PRO:HD3	1.82	0.42
1:H:235:THR:OG1	1:H:236:ARG:N	2.52	0.41
1:C:11:ILE:HD11	1:C:17:TRP:HZ2	1.85	0.41
1:D:176:ARG:O	1:D:212:THR:HA	2.19	0.41
1:G:192:PRO:O	1:G:193:MET:C	2.58	0.41
1:A:80:LEU:HG	1:A:80:LEU:O	2.20	0.41
1:G:129:VAL:HG23	1:G:130:PRO:HD2	2.01	0.41
1:L:68:TYR:CE2	1:L:84:LEU:HD13	2.55	0.41
1:H:189:GLY:O	1:H:196:PRO:HA	2.20	0.41
1:K:102:GLY:HA2	1:K:177:GLN:HG3	2.01	0.41
1:A:73:THR:O	1:A:76:ASP:HB2	2.20	0.41
1:G:176:ARG:HA	1:H:232:THR:CG2	2.50	0.41
1:F:49:HIS:ND1	1:F:49:HIS:N	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:GLU:CD	1:F:234:GLU:H	2.23	0.41
1:K:140:GLY:O	1:K:143:PRO:HD2	2.19	0.41
1:C:148:THR:O	1:C:152:LEU:HG	2.19	0.41
1:H:111:VAL:HG22	1:H:162:ASN:OD1	2.20	0.41
1:K:173:LEU:HD12	1:K:221:PHE:CB	2.50	0.41
1:J:182:TYR:OH	2:J:1202:PO4:O3	2.33	0.41
1:I:80:LEU:HG	1:I:84:LEU:HD12	2.01	0.41
1:K:234:GLU:H	1:K:234:GLU:CD	2.23	0.41
1:I:106:TRP:CD2	1:J:115:LYS:HE2	2.56	0.41
1:D:190:GLU:OE1	1:D:194:GLY:HA2	2.20	0.41
1:K:231:LEU:CD2	1:L:231:LEU:HD22	2.51	0.41
1:D:235:THR:C	1:D:237:LEU:H	2.24	0.41
1:E:210:GLU:HB2	1:E:215:TRP:CZ2	2.55	0.41
1:L:176:ARG:CB	1:L:176:ARG:CZ	2.99	0.41
1:E:102:GLY:C	1:E:177:GLN:HE21	2.23	0.41
1:F:129:VAL:HG22	1:F:130:PRO:HD2	2.02	0.41
1:C:95:VAL:CG1	1:C:129:VAL:HG12	2.51	0.41
1:J:94:GLY:HA3	1:J:95:VAL:HA	1.85	0.41
1:I:30:PHE:HB3	1:I:85:PHE:CD1	2.56	0.41
1:I:73:THR:O	1:I:76:ASP:HB2	2.21	0.41
1:I:49:HIS:HE1	1:I:76:ASP:OD1	2.04	0.41
1:F:197:PHE:HE1	1:F:199:TRP:CD1	2.39	0.41
1:K:129:VAL:O	1:K:129:VAL:HG13	2.21	0.41
1:K:144:TRP:CD2	1:K:169:PRO:HB2	2.55	0.41
1:G:134:GLU:HG2	1:G:167:LEU:CD1	2.51	0.41
1:A:7:ASN:C	1:A:7:ASN:OD1	2.58	0.41
1:K:159:PHE:CD1	1:K:159:PHE:C	2.94	0.41
1:A:173:LEU:HD23	1:A:174:TRP:O	2.21	0.41
1:A:69:ARG:NH1	1:A:71:ARG:HH11	2.10	0.41
1:L:106:TRP:CH2	1:L:231:LEU:HD13	2.56	0.41
1:C:165:LEU:HD12	1:C:165:LEU:H	1.85	0.41
1:L:142:ARG:HG2	1:L:142:ARG:HH11	1.86	0.41
1:L:132:ASN:HD22	1:L:132:ASN:HA	1.61	0.41
1:D:101:LEU:CD2	1:D:213:ASP:HB2	2.51	0.41
1:G:153:LEU:HD22	1:G:157:ARG:NH2	2.35	0.41
1:E:48:ALA:N	1:G:195:ARG:NH2	2.68	0.41
1:L:26:PHE:CD1	1:L:26:PHE:N	2.89	0.41
1:E:187:ILE:O	1:E:199:TRP:HB2	2.20	0.41
1:L:210:GLU:HA	1:L:215:TRP:CG	2.56	0.41
1:L:210:GLU:HG2	1:L:215:TRP:CE2	2.55	0.41
1:L:209:GLU:O	1:L:212:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:LEU:HD12	1:H:30:PHE:O	2.20	0.41
1:E:210:GLU:HA	1:E:215:TRP:CD2	2.56	0.41
1:F:80:LEU:HA	1:F:80:LEU:HD12	1.90	0.41
1:E:115:LYS:HE2	1:F:106:TRP:CD2	2.55	0.41
1:J:23:ALA:C	1:J:25:GLN:H	2.24	0.41
1:H:1:MET:CG	1:H:89:ASP:HB2	2.42	0.41
1:I:200:PHE:CD2	1:I:200:PHE:C	2.93	0.41
1:H:210:GLU:HA	1:H:215:TRP:CD2	2.56	0.41
1:B:166:PRO:HD2	1:B:222:VAL:HA	2.02	0.41
1:C:185:VAL:HB	1:C:201:ALA:O	2.21	0.41
1:A:96:ASN:ND2	1:A:100:ASN:HD21	2.19	0.41
1:H:176:ARG:O	1:H:212:THR:HA	2.21	0.40
1:H:131:LEU:HG	1:H:132:ASN:N	2.29	0.40
1:C:129:VAL:CG2	1:C:130:PRO:HD2	2.50	0.40
1:G:173:LEU:HD12	1:G:221:PHE:HD2	1.81	0.40
1:E:200:PHE:CD1	1:F:76:ASP:OD1	2.73	0.40
1:J:144:TRP:CE2	1:J:169:PRO:HB2	2.56	0.40
1:D:6:THR:O	1:D:93:SER:HA	2.21	0.40
1:G:207:GLU:HA	1:G:207:GLU:OE1	2.21	0.40
1:A:6:THR:O	1:A:93:SER:HA	2.21	0.40
1:C:100:ASN:OD1	1:C:108:SER:HB2	2.21	0.40
1:E:197:PHE:CD1	1:E:197:PHE:C	2.94	0.40
1:D:85:PHE:O	1:D:86:GLY:O	2.40	0.40
1:C:82:LEU:CD2	1:C:88:VAL:HB	2.51	0.40
1:B:118:TYR:HA	1:B:122:LEU:O	2.21	0.40
1:K:4:LEU:HB2	1:K:88:VAL:HG21	2.04	0.40
1:L:136:PRO:HA	1:L:167:LEU:CD2	2.52	0.40
1:J:206:LYS:HD2	1:J:206:LYS:O	2.22	0.40
1:H:155:LEU:HD21	1:H:174:TRP:CZ2	2.55	0.40
1:D:96:ASN:ND2	1:D:100:ASN:HD21	2.19	0.40
1:C:50:PRO:HA	1:D:198:TYR:O	2.22	0.40
1:L:23:ALA:HB3	1:L:29:VAL:HG21	2.04	0.40
1:E:236:ARG:NH1	1:F:158:PRO:O	2.54	0.40
1:F:210:GLU:HG2	1:F:215:TRP:CE2	2.56	0.40
1:D:63:PRO:O	1:D:64:HIS:C	2.60	0.40
1:I:147:ARG:NH1	1:I:151:THR:OG1	2.55	0.40
1:G:104:GLU:H	1:G:104:GLU:HG3	1.73	0.40
1:K:31:VAL:O	1:K:67:ALA:HA	2.20	0.40
1:J:53:ALA:CB	1:J:80:LEU:HD21	2.52	0.40
1:F:47:ILE:HD13	1:H:195:ARG:HH12	1.87	0.40
1:J:191:ASP:OD2	1:J:191:ASP:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:78:VAL:O	1:J:82:LEU:HG	2.21	0.40
1:J:91:VAL:O	1:J:124:ALA:HA	2.22	0.40
1:L:19:LEU:HD21	1:L:92:LEU:HB3	2.04	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	213/244 (87%)	198 (93%)	13 (6%)	2 (1%)	21 42
1	B	221/244 (91%)	198 (90%)	18 (8%)	5 (2%)	8 14
1	C	219/244 (90%)	202 (92%)	16 (7%)	1 (0%)	34 60
1	D	224/244 (92%)	201 (90%)	20 (9%)	3 (1%)	15 30
1	E	227/244 (93%)	215 (95%)	12 (5%)	0	100 100
1	F	222/244 (91%)	211 (95%)	9 (4%)	2 (1%)	21 42
1	G	225/244 (92%)	194 (86%)	24 (11%)	7 (3%)	5 8
1	H	225/244 (92%)	205 (91%)	17 (8%)	3 (1%)	15 30
1	I	221/244 (91%)	213 (96%)	7 (3%)	1 (0%)	34 60
1	J	216/244 (88%)	202 (94%)	12 (6%)	2 (1%)	21 42
1	K	220/244 (90%)	206 (94%)	13 (6%)	1 (0%)	34 60
1	L	225/244 (92%)	213 (95%)	9 (4%)	3 (1%)	15 30
All	All	2658/2928 (91%)	2458 (92%)	170 (6%)	30 (1%)	17 36

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	86	GLY

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Mol	Chain	Res	Type
1	G	132	ASN
1	G	209	GLU
1	H	173	LEU
1	J	206	LYS
1	K	132	ASN
1	A	193	MET
1	B	60	LEU
1	B	64	HIS
1	B	132	ASN
1	B	205	LEU
1	D	132	ASN
1	G	102	GLY
1	L	193	MET
1	C	86	GLY
1	D	236	ARG
1	H	48	ALA
1	F	132	ASN
1	F	192	PRO
1	G	87	PRO
1	H	24	SER
1	I	132	ASN
1	J	24	SER
1	G	122	LEU
1	D	86	GLY
1	L	133	GLY
1	A	194	GLY
1	B	143	PRO
1	G	62	ALA
1	L	194	GLY

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	176/194 (91%)	166 (94%)	10 (6%)	25 49
1	B	180/194 (93%)	173 (96%)	7 (4%)	39 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	181/194 (93%)	175 (97%)	6 (3%)	45 73
1	D	183/194 (94%)	177 (97%)	6 (3%)	45 73
1	E	187/194 (96%)	177 (95%)	10 (5%)	28 53
1	F	183/194 (94%)	174 (95%)	9 (5%)	31 57
1	G	184/194 (95%)	175 (95%)	9 (5%)	31 57
1	H	184/194 (95%)	175 (95%)	9 (5%)	31 57
1	I	182/194 (94%)	170 (93%)	12 (7%)	21 40
1	J	178/194 (92%)	174 (98%)	4 (2%)	60 83
1	K	182/194 (94%)	175 (96%)	7 (4%)	40 68
1	L	184/194 (95%)	174 (95%)	10 (5%)	27 52
All	All	2184/2328 (94%)	2085 (96%)	99 (4%)	34 62

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	49	HIS
1	A	97	LEU
1	A	176	ARG
1	A	187	ILE
1	A	200	PHE
1	A	206	LYS
1	A	217	VAL
1	A	235	THR
1	A	237	LEU
1	B	1	MET
1	B	60	LEU
1	B	80	LEU
1	B	89	ASP
1	B	106	TRP
1	B	196	PRO
1	B	206	LYS
1	C	52	ARG
1	C	65	PHE
1	C	156	GLU
1	C	173	LEU
1	C	176	ARG
1	C	234	GLU

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Mol	Chain	Res	Type
1	D	47	ILE
1	D	60	LEU
1	D	65	PHE
1	D	87	PRO
1	D	131	LEU
1	D	214	ARG
1	E	8	ASP
1	E	71	ARG
1	E	97	LEU
1	E	134	GLU
1	E	135	VAL
1	E	183	GLU
1	E	200	PHE
1	E	203	ARG
1	E	237	LEU
1	E	240	THR
1	F	131	LEU
1	F	147	ARG
1	F	168	ARG
1	F	203	ARG
1	F	206	LYS
1	F	214	ARG
1	F	219	GLN
1	F	234	GLU
1	F	238	GLN
1	G	28	GLU
1	G	35	ASP
1	G	82	LEU
1	G	107	HIS
1	G	118	TYR
1	G	131	LEU
1	G	134	GLU
1	G	147	ARG
1	G	206	LYS
1	H	1	MET
1	H	35	ASP
1	H	52	ARG
1	H	107	HIS
1	H	135	VAL
1	H	147	ARG
1	H	156	GLU
1	H	165	LEU

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Mol	Chain	Res	Type
1	H	173	LEU
1	I	28	GLU
1	I	60	LEU
1	I	107	HIS
1	I	123	SER
1	I	156	GLU
1	I	168	ARG
1	I	200	PHE
1	I	203	ARG
1	I	206	LYS
1	I	228	ARG
1	I	234	GLU
1	I	237	LEU
1	J	95	VAL
1	J	97	LEU
1	J	206	LYS
1	J	234	GLU
1	K	46	THR
1	K	47	ILE
1	K	65	PHE
1	K	74	PRO
1	K	87	PRO
1	K	147	ARG
1	K	200	PHE
1	L	36	THR
1	L	46	THR
1	L	52	ARG
1	L	97	LEU
1	L	132	ASN
1	L	173	LEU
1	L	193	MET
1	L	206	LYS
1	L	237	LEU
1	L	238	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	100	ASN
1	A	116	GLN
1	A	164	ASN

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Mol	Chain	Res	Type
1	A	219	GLN
1	B	56	HIS
1	B	96	ASN
1	B	132	ASN
1	B	164	ASN
1	B	177	GLN
1	C	7	ASN
1	C	116	GLN
1	C	164	ASN
1	D	100	ASN
1	D	116	GLN
1	D	164	ASN
1	D	177	GLN
1	E	116	GLN
1	E	164	ASN
1	E	238	GLN
1	F	164	ASN
1	F	177	GLN
1	F	238	GLN
1	G	49	HIS
1	G	96	ASN
1	G	164	ASN
1	G	177	GLN
1	H	49	HIS
1	H	56	HIS
1	H	164	ASN
1	H	177	GLN
1	I	49	HIS
1	I	116	GLN
1	I	164	ASN
1	I	177	GLN
1	I	219	GLN
1	J	56	HIS
1	J	116	GLN
1	J	132	ASN
1	J	164	ASN
1	K	100	ASN
1	K	116	GLN
1	K	132	ASN
1	K	164	ASN
1	L	116	GLN
1	L	132	ASN

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Mol	Chain	Res	Type
1	L	164	ASN
1	L	177	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)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	A	301	-	4,4,4	0.98	0	6,6,6	0.27	0
2	PO4	A	302	-	4,4,4	1.12	0	6,6,6	0.27	0
2	PO4	B	401	-	4,4,4	1.20	0	6,6,6	0.27	0
2	PO4	B	402	-	4,4,4	1.29	0	6,6,6	0.27	0
2	PO4	C	501	-	4,4,4	1.22	0	6,6,6	0.27	0
2	PO4	C	502	-	4,4,4	1.23	0	6,6,6	0.28	0
2	PO4	D	601	-	4,4,4	1.04	0	6,6,6	0.27	0
2	PO4	D	602	-	4,4,4	1.21	0	6,6,6	0.27	0
2	PO4	E	701	-	4,4,4	1.08	0	6,6,6	0.27	0
2	PO4	E	702	-	4,4,4	1.39	0	6,6,6	0.27	0
2	PO4	F	801	-	4,4,4	1.20	0	6,6,6	0.27	0
2	PO4	F	802	-	4,4,4	1.25	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PO4	G	901	-	4,4,4	1.01	0	6,6,6	0.27	0
2	PO4	G	902	-	4,4,4	1.20	0	6,6,6	0.27	0
2	PO4	H	1001	-	4,4,4	1.02	0	6,6,6	0.27	0
2	PO4	H	1002	-	4,4,4	1.24	0	6,6,6	0.27	0
2	PO4	I	1101	-	4,4,4	1.10	0	6,6,6	0.27	0
2	PO4	I	1102	-	4,4,4	1.22	0	6,6,6	0.27	0
2	PO4	J	1201	-	4,4,4	1.11	0	6,6,6	0.27	0
2	PO4	J	1202	-	4,4,4	1.11	0	6,6,6	0.27	0
2	PO4	J	1203	-	4,4,4	0.76	0	6,6,6	0.27	0
2	PO4	K	1301	-	4,4,4	0.96	0	6,6,6	0.28	0
2	PO4	K	1302	-	4,4,4	1.41	0	6,6,6	0.28	0
2	PO4	L	1401	-	4,4,4	1.18	0	6,6,6	0.27	0
2	PO4	L	1402	-	4,4,4	1.43	0	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	301	-	-	0/0/0/0	0/0/0/0
2	PO4	A	302	-	-	0/0/0/0	0/0/0/0
2	PO4	B	401	-	-	0/0/0/0	0/0/0/0
2	PO4	B	402	-	-	0/0/0/0	0/0/0/0
2	PO4	C	501	-	-	0/0/0/0	0/0/0/0
2	PO4	C	502	-	-	0/0/0/0	0/0/0/0
2	PO4	D	601	-	-	0/0/0/0	0/0/0/0
2	PO4	D	602	-	-	0/0/0/0	0/0/0/0
2	PO4	E	701	-	-	0/0/0/0	0/0/0/0
2	PO4	E	702	-	-	0/0/0/0	0/0/0/0
2	PO4	F	801	-	-	0/0/0/0	0/0/0/0
2	PO4	F	802	-	-	0/0/0/0	0/0/0/0
2	PO4	G	901	-	-	0/0/0/0	0/0/0/0
2	PO4	G	902	-	-	0/0/0/0	0/0/0/0
2	PO4	H	1001	-	-	0/0/0/0	0/0/0/0
2	PO4	H	1002	-	-	0/0/0/0	0/0/0/0
2	PO4	I	1101	-	-	0/0/0/0	0/0/0/0
2	PO4	I	1102	-	-	0/0/0/0	0/0/0/0
2	PO4	J	1201	-	-	0/0/0/0	0/0/0/0
2	PO4	J	1202	-	-	0/0/0/0	0/0/0/0
2	PO4	J	1203	-	-	0/0/0/0	0/0/0/0
2	PO4	K	1301	-	-	0/0/0/0	0/0/0/0
2	PO4	K	1302	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	L	1401	-	-	0/0/0/0	0/0/0/0
2	PO4	L	1402	-	-	0/0/0/0	0/0/0/0

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.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PO4	1	0
2	H	1001	PO4	1	0
2	H	1002	PO4	1	0
2	J	1202	PO4	2	0
2	K	1301	PO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	221/244 (90%)	-0.14	0 100 100	25, 50, 80, 107	0
1	B	225/244 (92%)	-0.15	4 (1%) 71 66	32, 54, 80, 112	0
1	C	225/244 (92%)	-0.05	5 (2%) 65 59	34, 56, 84, 112	0
1	D	228/244 (93%)	-0.24	3 (1%) 79 75	28, 46, 89, 110	0
1	E	233/244 (95%)	-0.29	1 (0%) 93 91	23, 44, 74, 103	0
1	F	228/244 (93%)	-0.32	2 (0%) 85 83	24, 43, 91, 106	0
1	G	229/244 (93%)	0.00	10 (4%) 38 30	32, 56, 90, 102	0
1	H	229/244 (93%)	-0.07	0 100 100	35, 57, 82, 104	0
1	I	227/244 (93%)	-0.40	1 (0%) 93 91	19, 40, 77, 91	0
1	J	222/244 (90%)	-0.27	2 (0%) 85 83	24, 47, 74, 100	0
1	K	226/244 (92%)	-0.31	2 (0%) 85 83	23, 40, 77, 101	0
1	L	229/244 (93%)	-0.29	4 (1%) 73 68	24, 39, 76, 103	0
All	All	2722/2928 (92%)	-0.21	34 (1%) 81 77	19, 48, 83, 112	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	205	LEU	4.1
1	G	60	LEU	3.9
1	L	192	PRO	3.6
1	G	193	MET	3.4
1	K	193	MET	3.3
1	L	61	HIS	3.2
1	L	36	THR	3.1
1	G	87	PRO	2.9
1	C	176	ARG	2.8
1	D	131	LEU	2.7
1	G	201	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	238	GLN	2.7
1	B	61	HIS	2.7
1	C	65	PHE	2.6
1	D	61	HIS	2.5
1	D	132	ASN	2.5
1	G	187	ILE	2.4
1	C	145	LEU	2.4
1	B	62	ALA	2.4
1	K	192	PRO	2.3
1	J	48	ALA	2.3
1	B	63	PRO	2.2
1	G	192	PRO	2.2
1	F	200	PHE	2.2
1	J	63	PRO	2.2
1	G	131	LEU	2.1
1	G	132	ASN	2.1
1	I	132	ASN	2.1
1	C	138	PHE	2.1
1	C	132	ASN	2.1
1	G	195	ARG	2.1
1	B	132	ASN	2.0
1	L	132	ASN	2.0
1	E	85	PHE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	L	1402	5/5	0.99	0.17	1.10	37,38,40,45	0
2	PO4	I	1102	5/5	0.99	0.16	0.72	38,40,43,49	0
2	PO4	J	1202	5/5	0.97	0.15	0.46	40,43,48,50	0
2	PO4	I	1101	5/5	0.99	0.14	0.12	19,23,37,38	0
2	PO4	F	802	5/5	0.99	0.14	0.08	32,35,37,39	0
2	PO4	B	402	5/5	0.99	0.14	0.07	46,47,49,52	0
2	PO4	K	1302	5/5	0.99	0.15	-0.12	39,40,48,49	0
2	PO4	E	701	5/5	0.98	0.13	-0.20	33,35,42,47	0
2	PO4	G	901	5/5	0.92	0.17	-0.27	54,55,68,69	0
2	PO4	D	602	5/5	0.98	0.14	-0.37	51,51,54,60	0
2	PO4	G	902	5/5	0.97	0.14	-0.65	69,70,73,76	0
2	PO4	L	1401	5/5	0.99	0.14	-0.67	31,31,36,39	0
2	PO4	H	1002	5/5	0.98	0.14	-0.72	35,44,49,56	0
2	PO4	A	302	5/5	0.97	0.15	-0.74	49,56,60,67	0
2	PO4	E	702	5/5	0.99	0.14	-0.80	38,39,48,49	0
2	PO4	D	601	5/5	0.96	0.11	-1.02	34,40,49,53	0
2	PO4	C	501	5/5	0.98	0.13	-1.25	45,47,52,56	0
2	PO4	F	801	5/5	0.99	0.09	-1.30	34,38,44,44	0
2	PO4	J	1201	5/5	0.99	0.10	-1.36	31,40,45,47	0
2	PO4	C	502	5/5	0.99	0.10	-1.38	42,44,50,59	0
2	PO4	A	301	5/5	0.97	0.10	-1.59	31,40,54,54	0
2	PO4	B	401	5/5	0.98	0.10	-1.74	38,44,49,52	0
2	PO4	K	1301	5/5	0.97	0.11	-2.18	29,41,48,49	0
2	PO4	H	1001	5/5	0.97	0.12	-2.40	28,35,52,52	0
2	PO4	J	1203	5/5	0.92	0.15	-	96,98,98,99	0

6.5 Other polymers (i)

There are no such residues in this entry.