Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:43 PM GMT

PDB ID	:	4MEX
Title	:	Crystal structure of Escherichia coli RNA polymerase in complex with salinamide A
Authors	:	Feng, Y.; Zhang, Y.; Arnold, E.; Ebright, R.H.
Deposited on	:	2013-08-27
Resolution	:	3.90 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 ⓘ symbol.

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

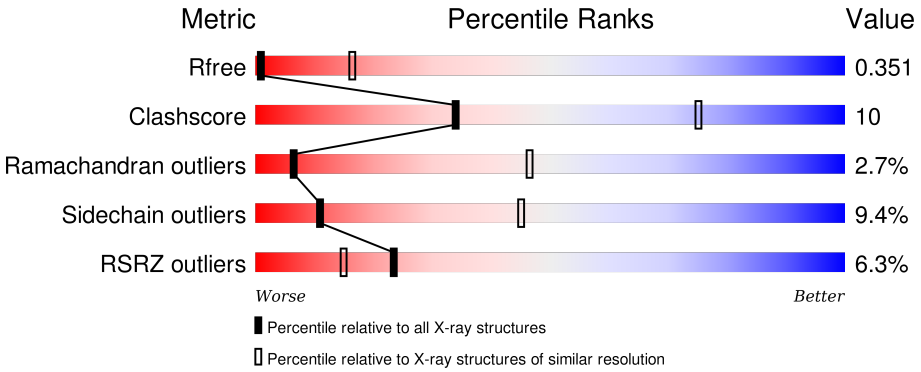
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.90 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	335	6% 65% 19% 11%
1	B	335	8% 56% 26% 14%
1	G	335	8% 44% 19% 36%
1	H	335	11% 45% 15% 36%
2	C	1342	5% 81% 17%

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Mol	Chain	Length	Quality of chain
2	I	1342	11% 79% 19%
3	D	1407	2% 62% 17% 18%
3	J	1407	2% 60% 19% 19%
4	E	91	79% 15%
4	K	91	5% 68% 14% 18%
5	F	613	5% 51% 22% 24%
5	L	613	5% 50% 22% 24%
6	M	9	78% 11% 11%
6	N	9	78% 11% 11%

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
6	D4P	M	4	-	-	X	-
6	MEA	M	5	-	-	X	-
6	2TL	M	6	-	-	X	-
6	D4P	N	4	-	-	X	-
6	MEA	N	5	-	-	X	-
6	2TL	N	6	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 50018 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2236	1405	391	432	8			
1	B	287	Total	C	N	O	S	0	0	0
			2160	1359	374	419	8			
1	G	216	Total	C	N	O	S	0	0	0
			1618	1013	282	317	6			
1	H	215	Total	C	N	O	S	0	0	0
			1605	1005	278	316	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	3	0	0
			9522	5999	1675	1829	19			
2	I	1340	Total	C	N	O	S	3	0	0
			9544	6013	1676	1835	20			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1150	Total	C	N	O	S	0	0	0
			7572	4771	1358	1415	28			
3	J	1143	Total	C	N	O	S	0	0	0
			7535	4748	1351	1408	28			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	0	0	0
			482	299	93	90			
4	K	75	Total	C	N	O	0	0	0
			408	253	79	76			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	464	Total	C	N	O	S	0	0	0
			3592	2253	643	682	14			
5	L	464	Total	C	N	O	S	0	0	0
			3592	2253	643	682	14			

- Molecule 6 is a protein called Salinamide A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	9	Total	C	N	O	0	0	0
			73	51	7	15			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	N	9	Total C N O 73 51 7 15	0	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

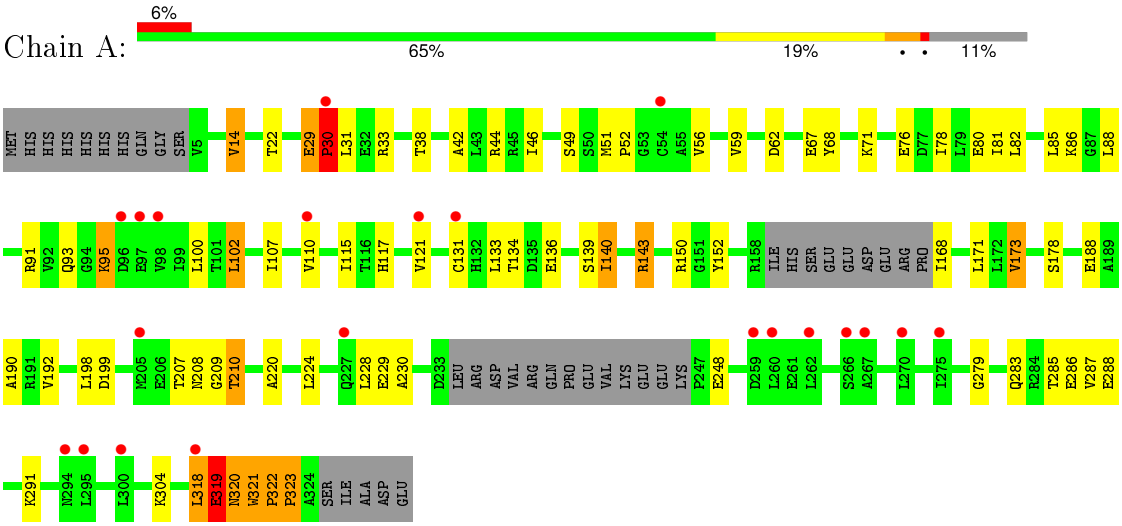
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	J	2	Total Zn 2 2	0	0
8	D	2	Total Zn 2 2	0	0

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.

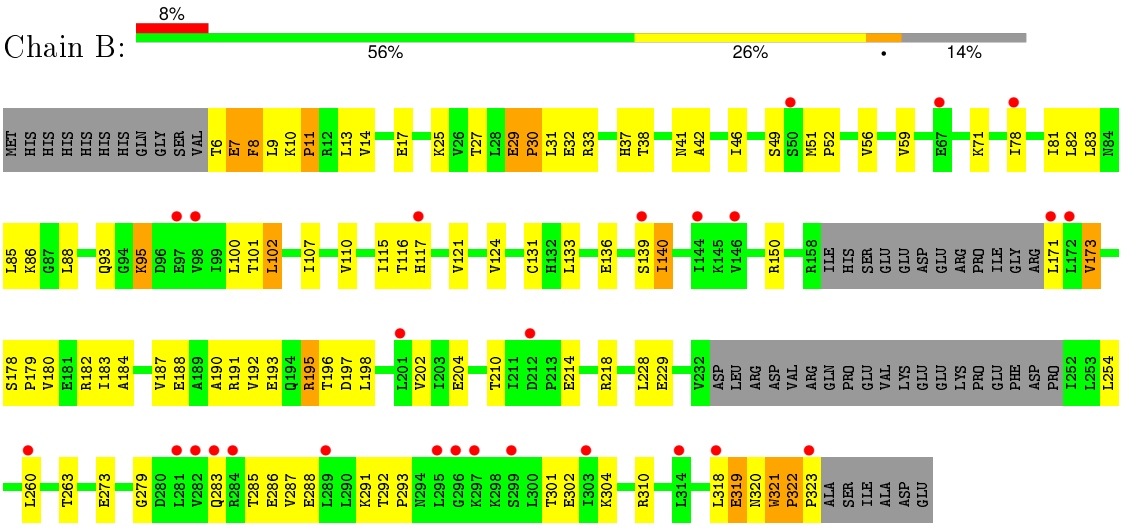
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



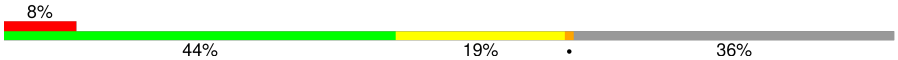
- Molecule 1: DNA-directed RNA polymerase subunit alpha

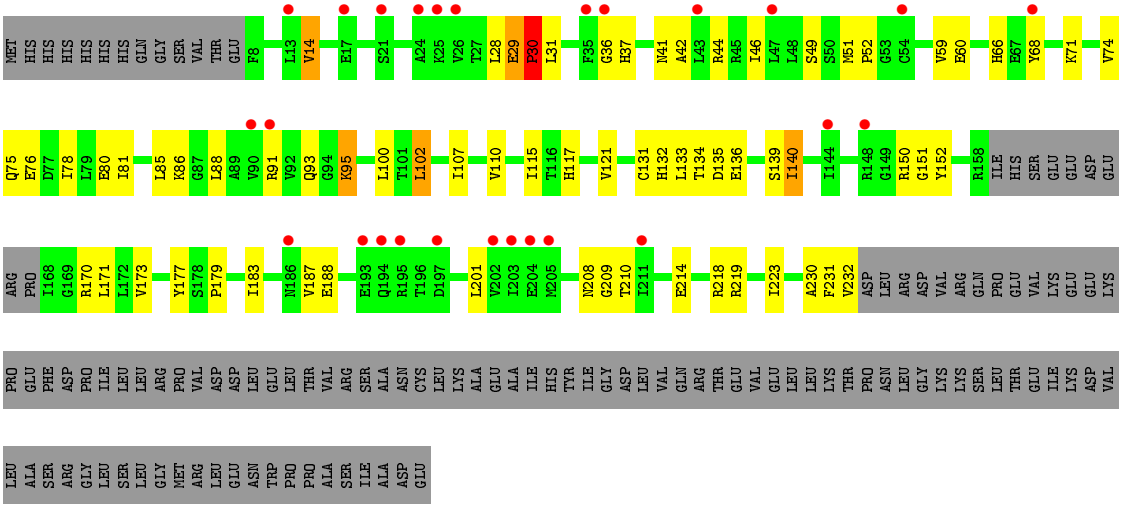
Chain B:



- Molecule 1: DNA-directed RNA polymerase subunit alpha

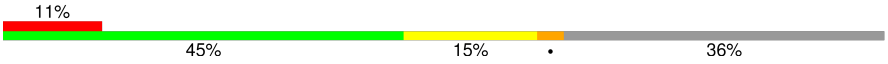
Chain G:

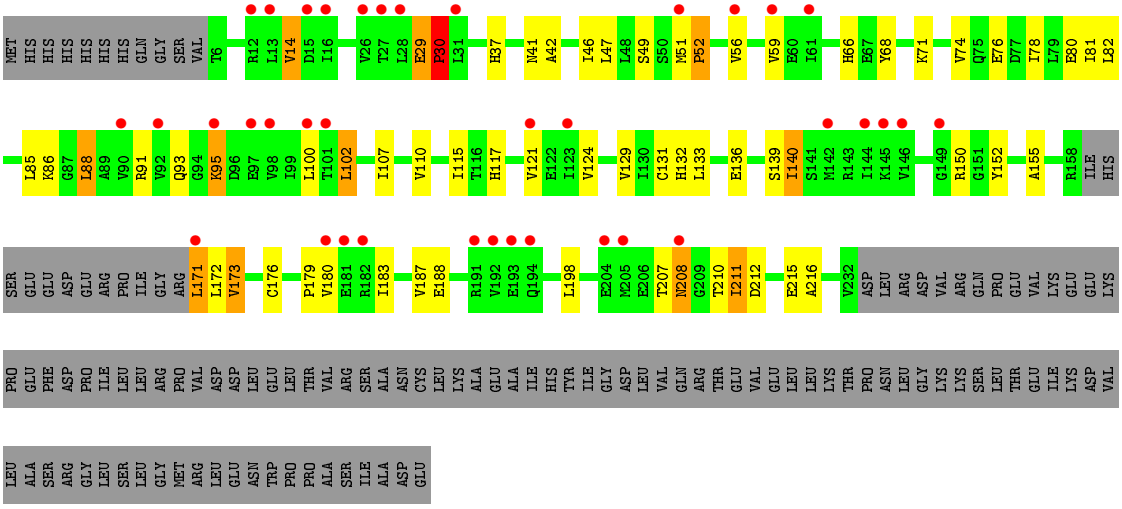




• Molecule 1: DNA-directed RNA polymerase subunit alpha

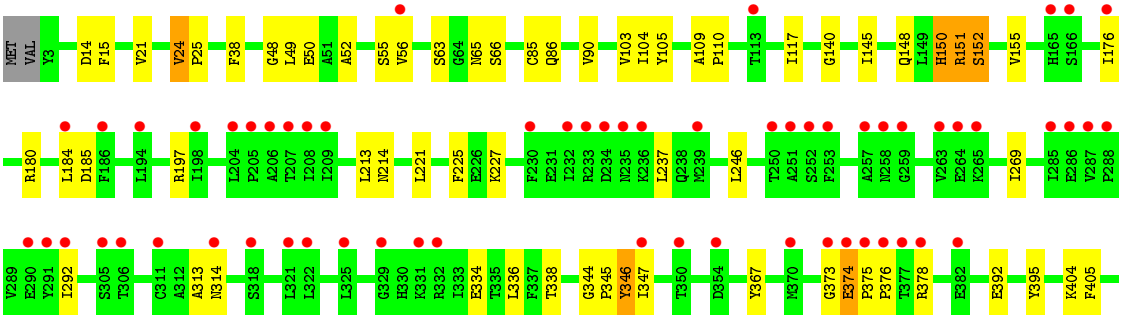
Chain H:

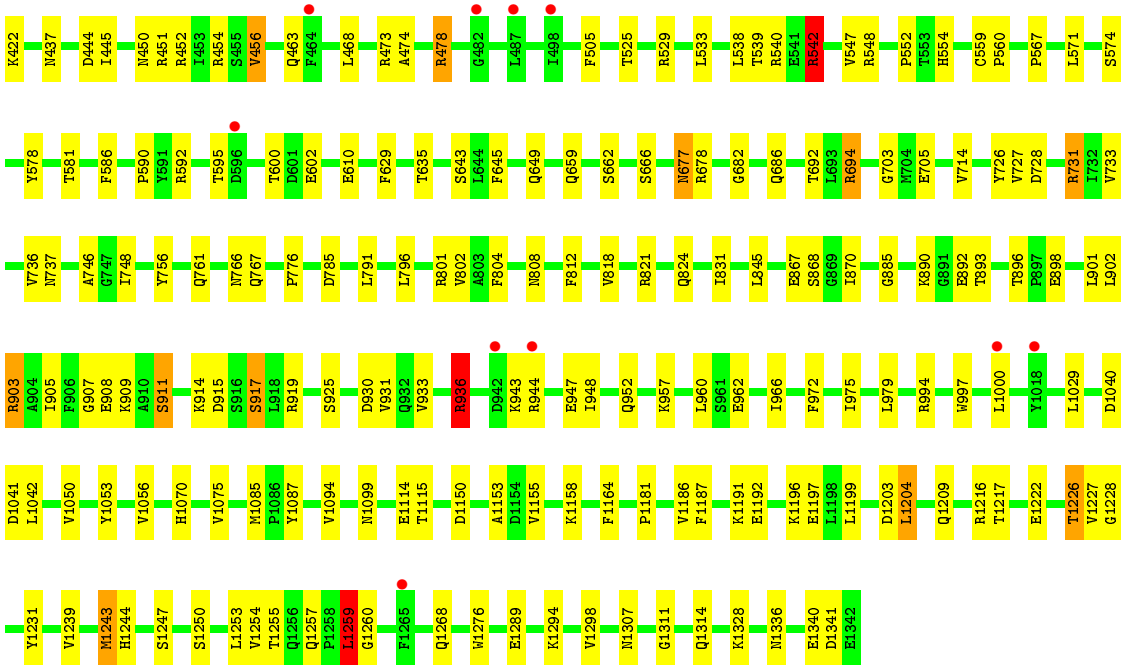




• Molecule 2: DNA-directed RNA polymerase subunit beta

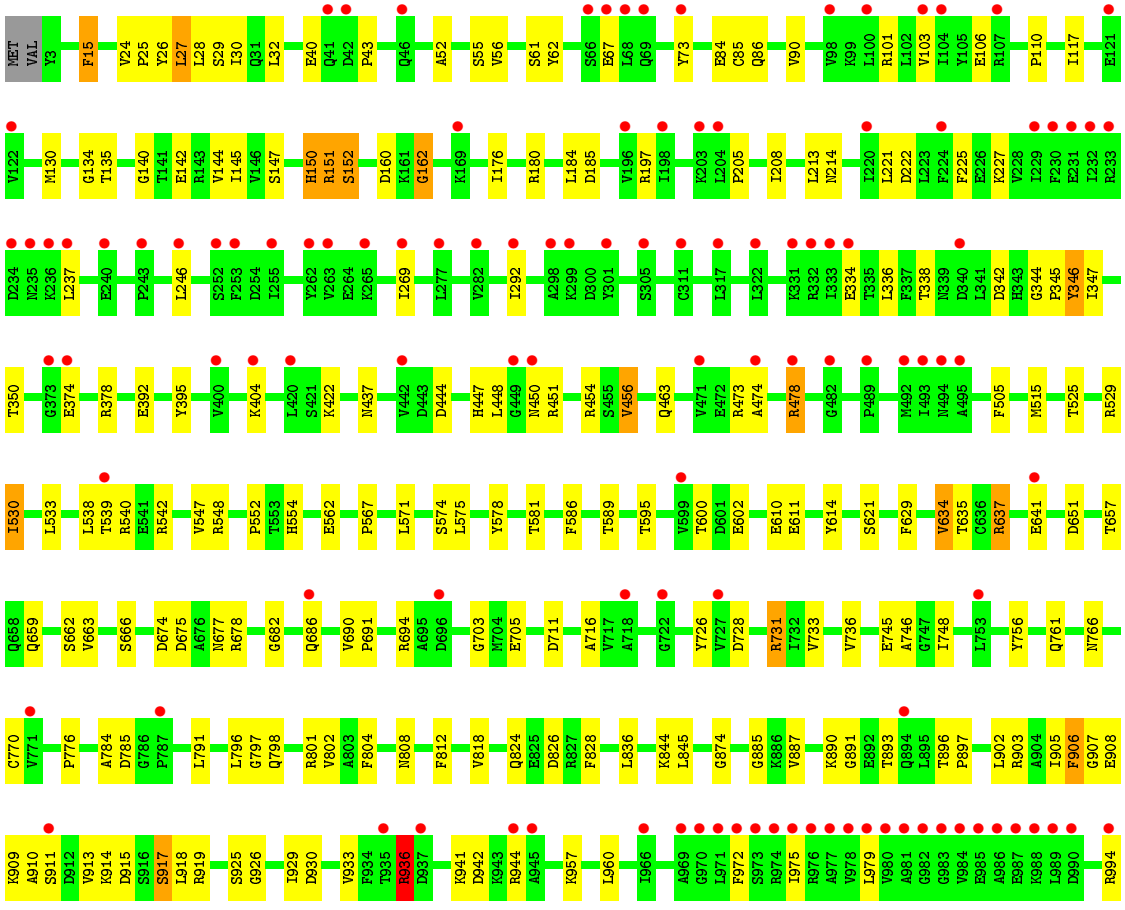
Chain C:

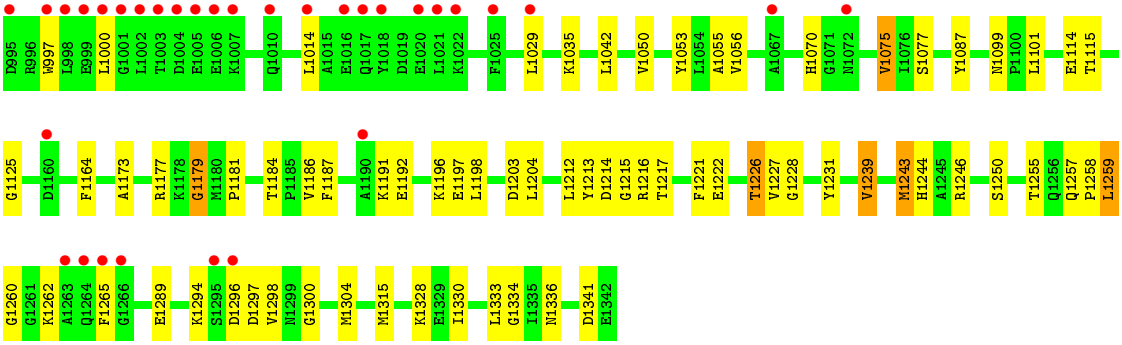




• Molecule 2: DNA-directed RNA polymerase subunit beta

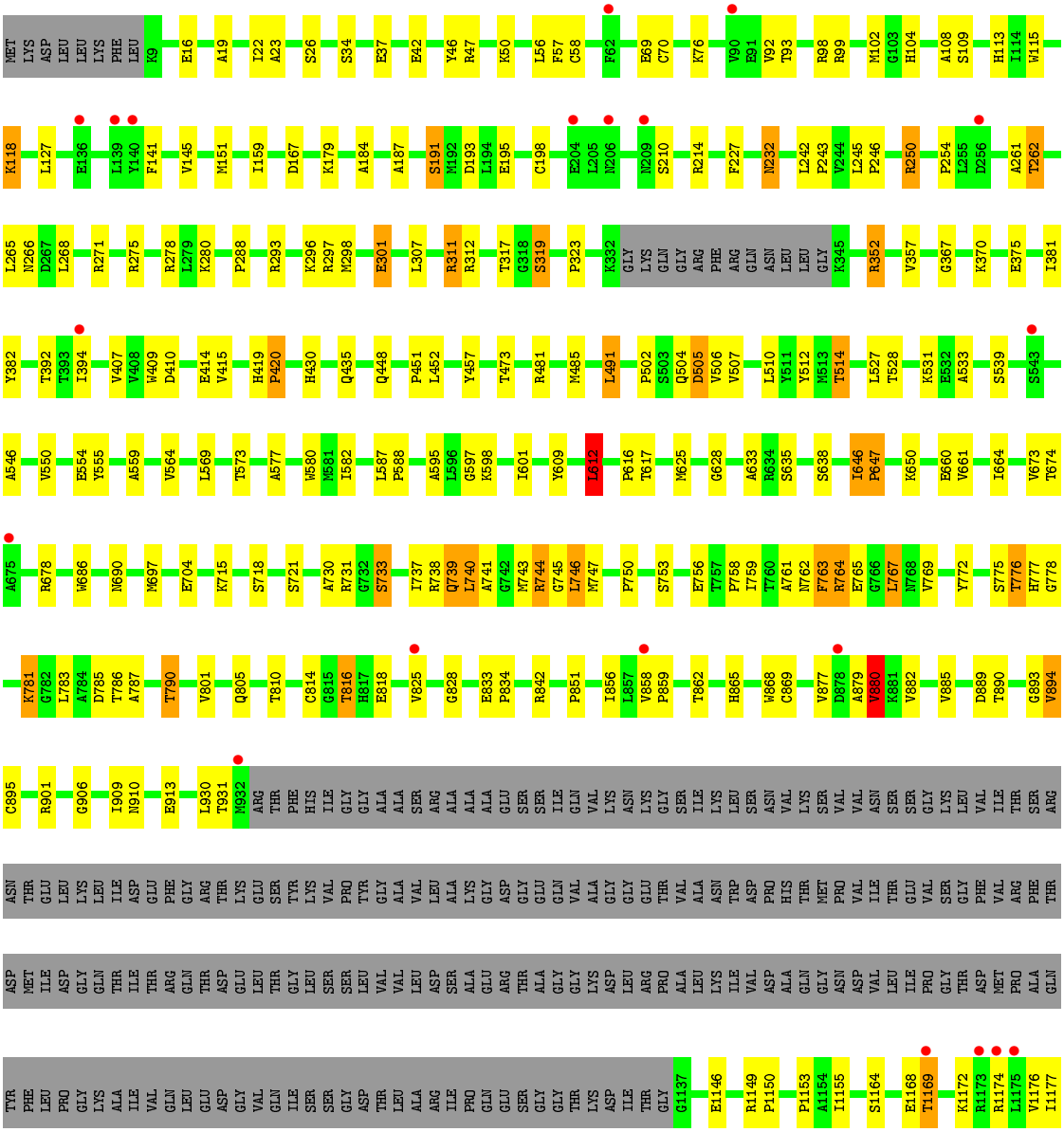
Chain I:

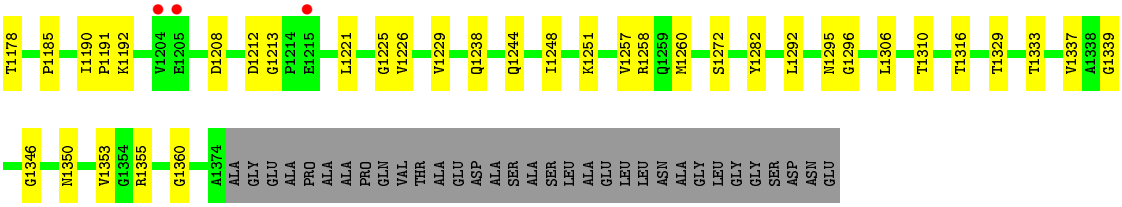


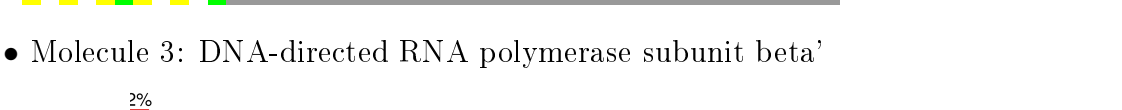


- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:

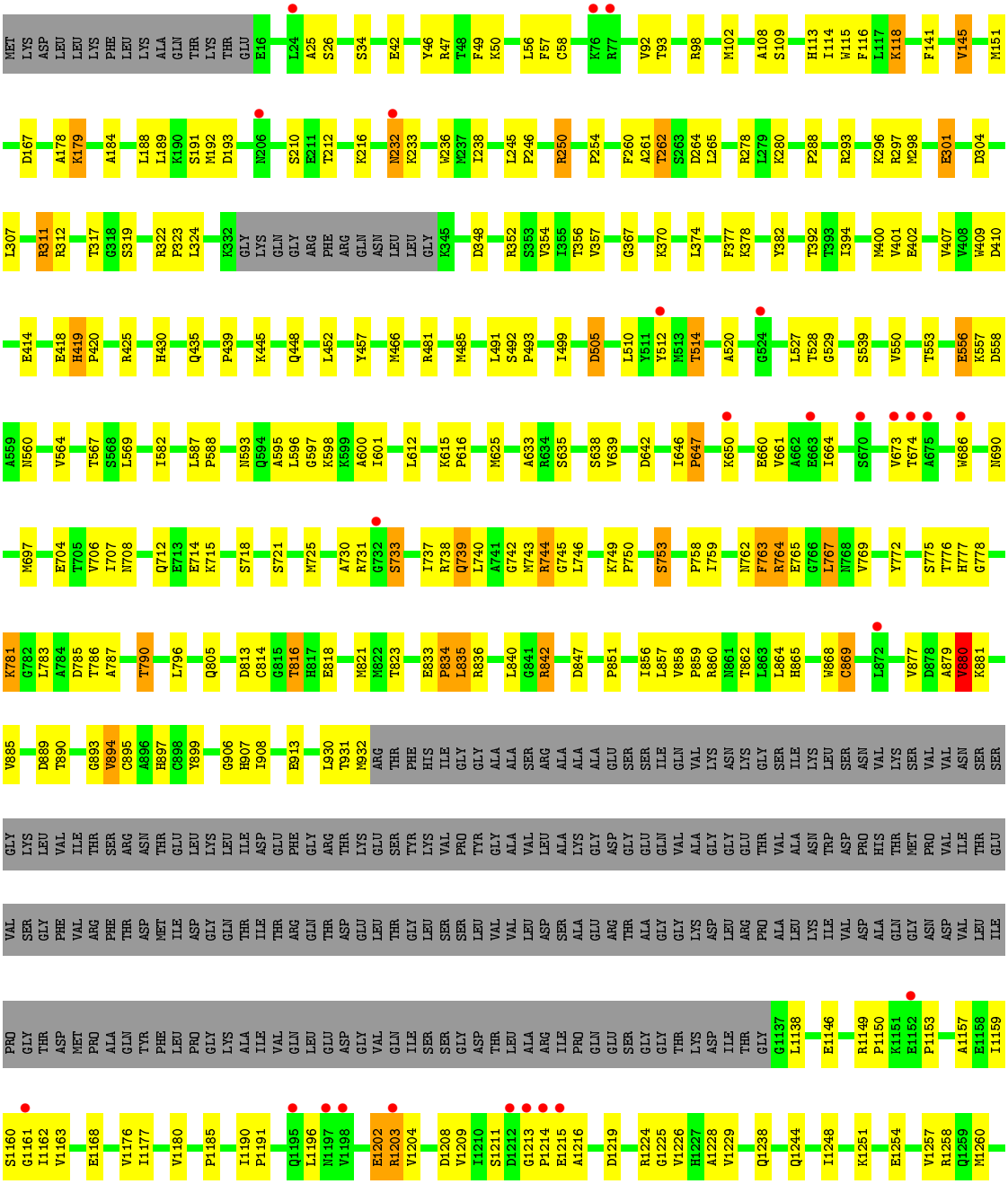


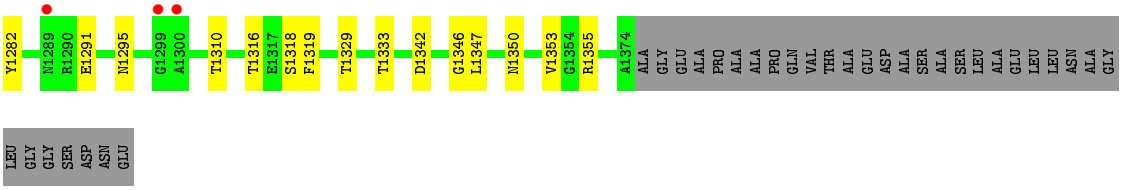




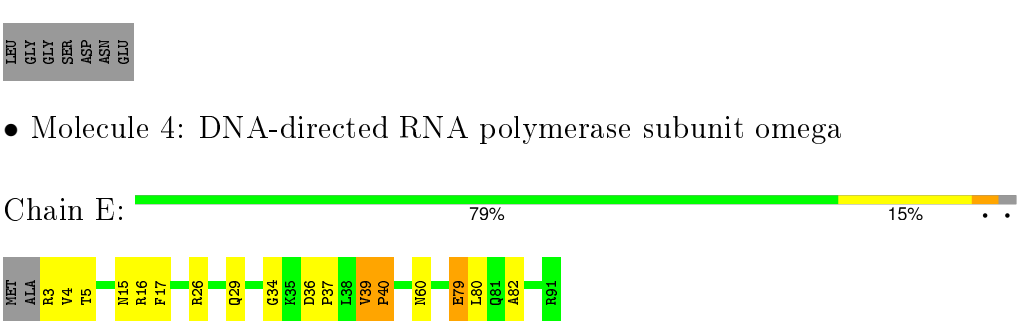
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J:

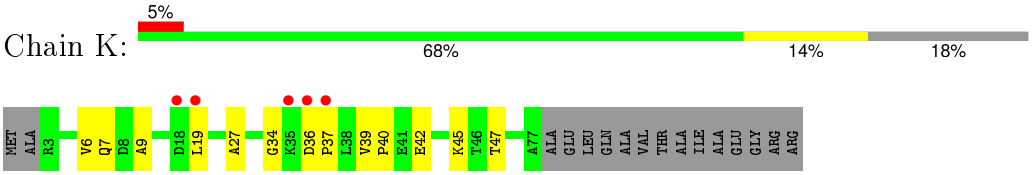




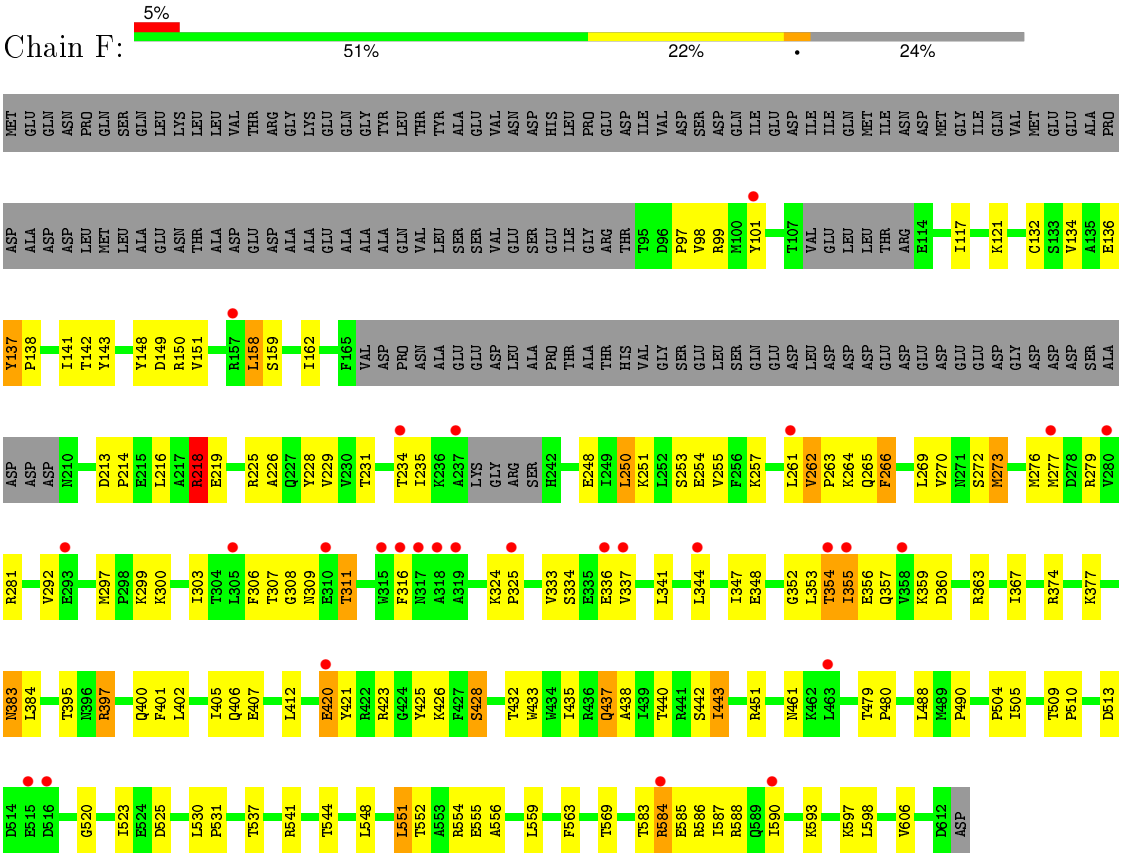
• Molecule 4: DNA-directed RNA polymerase subunit omega



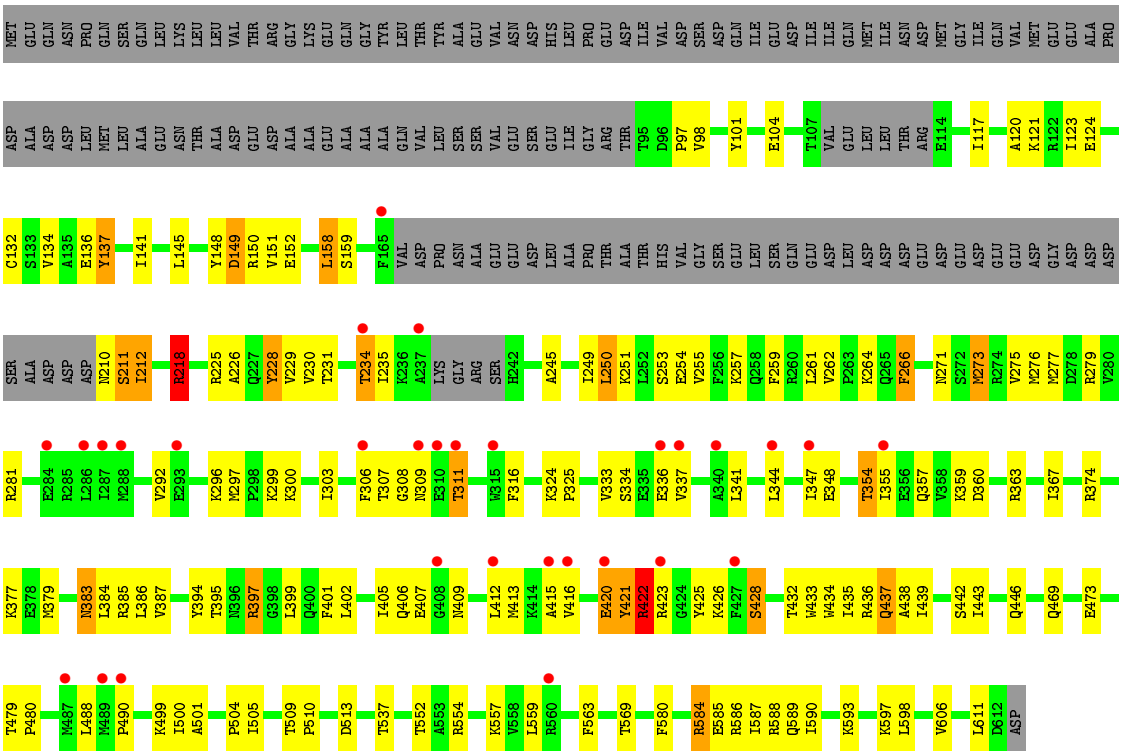
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 5: RNA polymerase sigma factor RpoD

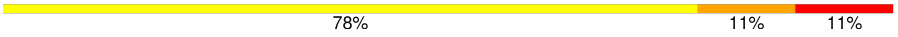


- Molecule 6: Salinamide A

Chain M:

- Molecule 6: Salinamide A

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	185.80Å 208.19Å 308.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 3.90 49.87 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.87-3.90) 97.6 (49.87-3.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.286 , 0.325 0.313 , 0.351	Depositor DCC
R_{free} test set	2174 reflections (2.08%)	DCC
Wilson B-factor (Å^2)	151.0	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 156.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 108751 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	50018	wwPDB-VP
Average B, all atoms (Å^2)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: 28H, MG, 28J, MEA, 2TL, ZN, 28K, D4P

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	0.25	0/2263	0.55	1/3073 (0.0%)
1	B	0.26	0/2185	0.58	0/2967
1	G	0.25	0/1636	0.55	0/2221
1	H	0.28	0/1623	0.53	0/2205
2	C	0.24	0/9653	0.50	3/13062 (0.0%)
2	I	0.24	0/9676	0.48	1/13089 (0.0%)
3	D	0.24	0/7667	0.51	1/10416 (0.0%)
3	J	0.24	0/7630	0.51	0/10365
4	E	0.25	0/482	0.68	1/662 (0.2%)
4	K	0.26	0/407	0.57	0/558
5	F	0.26	0/3636	0.54	2/4892 (0.0%)
5	L	0.26	0/3636	0.55	3/4892 (0.1%)
6	M	2.92	3/14 (21.4%)	0.80	0/14
6	N	2.92	3/14 (21.4%)	0.79	0/14
All	All	0.26	6/50522 (0.0%)	0.52	12/68430 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	8	GLY	CA-C	-7.75	1.39	1.51
6	N	8	GLY	CA-C	-7.73	1.39	1.51
6	M	2	THR	CA-C	-5.17	1.39	1.52
6	N	2	THR	CA-C	-5.17	1.39	1.52
6	M	7	SER	CA-C	-5.16	1.39	1.52
6	N	7	SER	CA-C	-5.16	1.39	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	39	VAL	C-N-CA	7.85	154.96	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	612	LEU	CA-CB-CG	7.73	133.07	115.30
2	I	936	ARG	NE-CZ-NH2	6.61	123.61	120.30
5	F	218	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	C	936	ARG	NE-CZ-NH2	6.26	123.43	120.30
5	L	218	ARG	NE-CZ-NH1	6.09	123.35	120.30
2	C	1259	LEU	CA-CB-CG	5.41	127.73	115.30
5	L	422	ARG	NE-CZ-NH1	5.29	122.94	120.30
5	F	149	ASP	CB-CG-OD2	5.22	123.00	118.30
5	L	149	ASP	CB-CG-OD2	5.22	122.99	118.30
1	A	318	LEU	CA-CB-CG	5.07	126.96	115.30
2	C	542	ARG	NE-CZ-NH2	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	2236	0	2254	49	0
1	B	2160	0	2184	59	1
1	G	1618	0	1622	41	0
1	H	1605	0	1599	44	1
2	C	9522	0	8569	149	0
2	I	9544	0	8601	156	0
3	D	7572	0	6293	156	0
3	J	7535	0	6272	162	0
4	E	482	0	301	7	0
4	K	408	0	255	4	0
5	F	3592	0	3433	89	1
5	L	3592	0	3433	94	1
6	M	73	0	64	34	0
6	N	73	0	64	31	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	50018	0	44944	955	2

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 10.

All (955) 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)
6:N:4:D4P:C4	6:N:9:28K:H46	1.64	1.26
6:M:4:D4P:C4	6:M:9:28K:H46	1.64	1.25
6:N:4:D4P:C3	6:N:9:28K:H46	1.68	1.22
6:M:4:D4P:C5	6:M:9:28K:H46	1.68	1.22
6:M:4:D4P:C4	6:M:9:28K:CAF	2.37	0.99
2:C:936:ARG:HH21	2:C:936:ARG:HG3	1.29	0.98
2:I:936:ARG:HH21	2:I:936:ARG:HG3	1.27	0.96
6:N:4:D4P:C3	6:N:9:28K:CAF	2.45	0.95
6:M:4:D4P:C5	6:M:9:28K:CAF	2.45	0.94
6:N:4:D4P:C4	6:N:9:28K:CAF	2.37	0.92
3:D:745:GLY:HA3	6:M:1:28H:H11	1.56	0.88
3:J:744:ARG:NH2	3:J:767:LEU:HD21	1.89	0.87
3:J:745:GLY:HA3	6:N:1:28H:H11	1.56	0.87
1:G:44:ARG:NH2	2:I:1087:TYR:OH	2.07	0.85
6:M:1:28H:H5	6:M:3:28J:H22	1.58	0.84
1:H:29:GLU:HG3	1:H:30:PRO:HD2	1.61	0.83
6:N:1:28H:H5	6:N:3:28J:H22	1.58	0.83
1:B:10:LYS:HB3	1:B:11:PRO:HD2	1.61	0.83
1:H:51:MET:HB3	1:H:179:PRO:HD2	1.60	0.83
1:B:182:ARG:HD3	3:D:531:LYS:HA	1.59	0.82
5:L:587:ILE:HD12	5:L:590:ILE:HD11	1.63	0.81
3:J:527:LEU:O	3:J:529:GLY:N	2.14	0.80
3:J:118:LYS:HE3	3:J:312:ARG:HG3	1.63	0.80
5:F:587:ILE:HD12	5:F:590:ILE:HD11	1.63	0.80
1:G:14:VAL:HG11	1:G:29:GLU:HG3	1.65	0.79
2:C:808:ASN:H	3:D:633:ALA:HB2	1.48	0.79
1:A:228:LEU:O	1:A:230:ALA:N	2.14	0.78
3:D:781:LYS:HB3	6:M:5:MEA:CE1	2.14	0.78
3:J:739:GLN:HA	3:J:739:GLN:OE1	1.84	0.77
2:I:345:PRO:O	2:I:347:ILE:N	2.17	0.77
5:F:218:ARG:HH11	5:F:218:ARG:HG2	1.50	0.77
2:C:345:PRO:O	2:C:347:ILE:N	2.18	0.77
3:J:744:ARG:HH21	3:J:767:LEU:HD21	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:2:THR:HG21	6:N:6:2TL:O	1.86	0.76
2:I:637:ARG:HG3	2:I:641:GLU:HA	1.69	0.75
5:L:399:LEU:HD13	5:L:446:GLN:HG2	1.68	0.75
6:M:2:THR:HG21	6:M:6:2TL:O	1.86	0.75
3:D:738:ARG:HH22	6:M:1:28H:H6	1.51	0.74
3:D:739:GLN:HA	3:D:739:GLN:OE1	1.87	0.74
3:D:746:LEU:HD22	3:D:758:PRO:HB3	1.68	0.74
3:J:738:ARG:HH22	6:N:1:28H:H6	1.52	0.74
3:J:262:THR:HG22	5:L:504:PRO:HB2	1.69	0.74
2:C:65:ASN:O	2:C:105:TYR:N	2.21	0.73
1:G:60:GLU:HG3	1:G:170:ARG:HD2	1.69	0.73
3:D:781:LYS:HB3	6:M:5:MEA:CD1	2.19	0.73
1:B:110:VAL:HG21	1:B:140:ILE:HD11	1.71	0.73
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.71	0.72
1:A:208:ASN:OD1	1:A:210:THR:OG1	2.06	0.72
1:H:91:ARG:NH2	1:H:210:THR:O	2.22	0.72
2:C:885:GLY:HA2	2:C:917:SER:HB3	1.72	0.71
1:H:110:VAL:HG21	1:H:140:ILE:HD11	1.73	0.71
3:D:262:THR:HG22	5:F:504:PRO:HB2	1.73	0.71
3:J:377:PHE:HE1	3:J:419:HIS:HD1	1.38	0.71
3:J:288:PRO:HA	5:L:377:LYS:HE3	1.73	0.71
1:A:91:ARG:NH2	1:A:209:GLY:O	2.24	0.70
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.74	0.70
2:I:222:ASP:OD1	2:I:227:LYS:NZ	2.23	0.70
1:H:86:LYS:HG2	1:H:173:VAL:HG23	1.74	0.70
1:G:110:VAL:HG21	1:G:140:ILE:HD11	1.74	0.69
1:B:30:PRO:HD3	1:B:190:ALA:HB1	1.72	0.69
1:A:150:ARG:HH21	1:B:6:THR:HA	1.57	0.69
3:D:744:ARG:HB3	3:D:759:ILE:HB	1.76	0.68
5:F:134:VAL:HG11	5:F:266:PHE:HE1	1.58	0.68
5:L:152:GLU:OE2	5:L:218:ARG:NH1	2.26	0.68
2:C:1099:ASN:ND2	3:D:505:ASP:OD2	2.25	0.68
3:J:245:LEU:O	3:J:250:ARG:NH1	2.26	0.68
3:J:118:LYS:HB3	3:J:311:ARG:HD2	1.75	0.68
3:J:781:LYS:HB3	6:N:5:MEA:CE1	2.23	0.68
3:D:118:LYS:HE3	3:D:312:ARG:HG3	1.75	0.68
3:D:781:LYS:HB3	6:M:5:MEA:HE1	1.75	0.67
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.75	0.67
2:I:548:ARG:NH2	2:I:567:PRO:O	2.26	0.67
2:I:1099:ASN:ND2	3:J:505:ASP:OD2	2.26	0.67
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:744:ARG:HB3	3:J:759:ILE:HB	1.76	0.67
5:L:218:ARG:HH11	5:L:218:ARG:HG2	1.58	0.67
6:M:4:D4P:C3	6:M:9:28K:H46	2.23	0.67
1:A:110:VAL:HG21	1:A:140:ILE:HD11	1.76	0.67
2:I:915:ASP:OD1	2:I:917:SER:OG	2.12	0.67
2:I:915:ASP:OD2	2:I:919:ARG:NH2	2.27	0.67
3:J:114:ILE:HD12	3:J:114:ILE:H	1.60	0.67
2:I:30:ILE:HD12	2:I:575:LEU:HD22	1.77	0.66
2:I:86:GLN:HA	2:I:140:GLY:HA2	1.77	0.66
2:C:890:LYS:HG2	2:C:914:LYS:HG3	1.78	0.66
3:D:57:PHE:O	3:D:98:ARG:NH2	2.28	0.66
2:C:915:ASP:OD1	2:C:917:SER:OG	2.14	0.66
2:C:344:GLY:H	2:C:437:ASN:ND2	1.92	0.66
1:G:133:LEU:HD21	1:G:140:ILE:HG12	1.78	0.65
2:C:548:ARG:NH2	2:C:567:PRO:O	2.30	0.65
5:F:98:VAL:HG22	5:F:402:LEU:HD13	1.79	0.65
2:I:26:TYR:HB2	2:I:29:SER:HB3	1.77	0.65
2:C:694:ARG:HG3	2:C:694:ARG:HH11	1.60	0.65
5:F:162:ILE:HG22	5:F:261:LEU:HD23	1.79	0.65
1:G:91:ARG:NH2	1:G:209:GLY:O	2.30	0.65
2:I:621:SER:HB2	2:I:629:PHE:CE1	2.32	0.65
1:H:78:ILE:HD13	1:H:81:ILE:HD12	1.78	0.64
3:D:865:HIS:HB3	3:D:868:TRP:HD1	1.61	0.64
2:C:796:LEU:N	2:C:1231:TYR:OH	2.29	0.64
6:N:4:D4P:C5	6:N:9:28K:H46	2.23	0.64
6:M:1:28H:OCD	6:M:1:28H:H6	1.97	0.64
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.80	0.64
2:I:1196:LYS:NZ	3:J:642:ASP:OD2	2.30	0.64
3:J:370:LYS:HB3	3:J:409:TRP:CZ3	2.33	0.64
2:I:444:ASP:O	2:I:450:ASN:ND2	2.28	0.64
6:N:1:28H:OCD	6:N:1:28H:H6	1.97	0.64
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.79	0.64
5:F:405:ILE:HD12	5:F:406:GLN:HE21	1.61	0.64
2:I:890:LYS:HG2	2:I:914:LYS:HB2	1.80	0.64
2:C:21:VAL:HG21	2:C:592:ARG:HD3	1.79	0.64
2:C:1186:VAL:HG13	2:C:1187:PHE:HD1	1.63	0.64
2:I:936:ARG:NH2	2:I:936:ARG:HG3	2.03	0.64
2:I:1186:VAL:HG13	2:I:1187:PHE:HD1	1.63	0.64
3:D:288:PRO:HA	5:F:377:LYS:HE3	1.80	0.63
4:E:26:ARG:NH1	4:E:29:GLN:OE1	2.31	0.63
3:J:1146:GLU:OE2	3:J:1310:THR:OG1	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:897:PRO:HB3	5:L:563:PHE:O	1.98	0.63
1:A:287:VAL:HG12	1:A:291:LYS:HE3	1.78	0.63
2:I:28:LEU:O	2:I:32:LEU:N	2.28	0.63
3:J:686:TRP:HB3	3:J:746:LEU:HD21	1.81	0.63
4:E:3:ARG:O	4:E:5:THR:N	2.31	0.63
5:L:124:GLU:OE1	5:L:422:ARG:NH1	2.29	0.63
6:M:4:D4P:C6	6:M:9:28K:H46	2.29	0.62
5:L:422:ARG:CG	5:L:422:ARG:HH11	2.12	0.62
3:D:250:ARG:O	3:D:266:ASN:ND2	2.30	0.62
3:J:1157:ALA:HB3	3:J:1208:ASP:HA	1.80	0.62
1:G:66:HIS:HB3	2:I:874:GLY:HA2	1.80	0.62
1:G:59:VAL:HG21	1:G:85:LEU:HD13	1.79	0.62
2:I:344:GLY:H	2:I:437:ASN:HD21	1.45	0.62
3:J:114:ILE:HD13	3:J:307:LEU:HB2	1.80	0.62
2:I:629:PHE:CE2	2:I:634:VAL:HG12	2.33	0.62
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.82	0.62
1:H:37:HIS:CE1	1:H:187:VAL:HG21	2.34	0.62
2:C:1268:GLN:NE2	3:D:352:ARG:HB3	2.14	0.62
3:J:781:LYS:HB3	6:N:5:MEA:HE1	1.81	0.62
3:D:739:GLN:HE22	3:D:744:ARG:HG3	1.65	0.62
3:D:102:MET:HG2	3:D:246:PRO:HD3	1.80	0.62
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.79	0.62
6:M:2:THR:HG23	6:M:6:2TL:HB	1.82	0.62
2:C:56:VAL:HG21	2:C:468:LEU:HB3	1.82	0.62
3:J:317:THR:HA	3:J:323:PRO:HA	1.81	0.62
3:J:739:GLN:HE22	3:J:744:ARG:HG3	1.65	0.62
1:B:29:GLU:HB3	1:B:30:PRO:HD2	1.82	0.62
3:J:1162:ILE:O	3:J:1180:VAL:N	2.26	0.62
1:G:51:MET:HB3	1:G:179:PRO:HG2	1.82	0.62
2:C:542:ARG:HG2	2:C:542:ARG:HH21	1.65	0.62
1:A:133:LEU:HD21	1:A:140:ILE:HG12	1.80	0.61
2:C:677:ASN:HD22	2:C:677:ASN:H	1.46	0.61
1:H:208:ASN:HB3	1:H:210:THR:HG23	1.82	0.61
5:L:211:SER:OG	5:L:212:ILE:N	2.33	0.61
3:J:1162:ILE:HA	3:J:1203:ARG:HA	1.82	0.61
2:C:931:VAL:HB	2:C:944:ARG:HH22	1.64	0.61
1:B:37:HIS:CE1	1:B:187:VAL:HG21	2.35	0.61
3:D:370:LYS:HB3	3:D:409:TRP:CZ3	2.35	0.61
2:I:614:TYR:HB3	2:I:651:ASP:HB2	1.82	0.61
3:D:930:LEU:HA	3:D:1244:GLN:HG3	1.81	0.61
1:B:184:ALA:HB3	1:B:204:GLU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:344:GLY:H	2:C:437:ASN:HD21	1.48	0.61
1:H:211:ILE:HD11	1:H:216:ALA:HB2	1.82	0.61
6:N:4:D4P:C2	6:N:9:28K:H46	2.29	0.61
2:I:1304:MET:HA	2:I:1315:MET:HB3	1.81	0.61
1:B:41:ASN:HD21	2:C:1217:THR:HG22	1.66	0.61
6:N:2:THR:HG23	6:N:6:2TL:CB	2.31	0.61
5:L:354:THR:HG22	5:L:357:GLN:HE21	1.64	0.61
6:N:2:THR:HG23	6:N:6:2TL:HB	1.82	0.61
1:B:29:GLU:CB	1:B:30:PRO:HD2	2.31	0.61
2:C:933:VAL:HG13	2:C:1050:VAL:HG22	1.83	0.61
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.31	0.61
3:D:118:LYS:HB3	3:D:311:ARG:HD2	1.82	0.60
1:A:71:LYS:NZ	1:A:139:SER:O	2.34	0.60
2:I:147:SER:HB2	2:I:530:ILE:HG22	1.81	0.60
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.83	0.60
4:K:9:ALA:HB1	4:K:19:LEU:HD21	1.83	0.60
2:C:151:ARG:HH21	2:C:445:ILE:HD13	1.66	0.60
3:D:745:GLY:CA	6:M:1:28H:H11	2.31	0.60
1:B:287:VAL:HG12	1:B:291:LYS:HE3	1.82	0.60
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.33	0.60
6:M:2:THR:HG23	6:M:6:2TL:CB	2.31	0.60
3:J:57:PHE:O	3:J:98:ARG:NH2	2.35	0.60
3:J:452:LEU:HG	3:J:625:MET:HE3	1.83	0.60
6:N:5:MEA:C	6:N:7:SER:N	2.65	0.60
2:I:796:LEU:N	2:I:1231:TYR:OH	2.33	0.60
2:C:148:GLN:NE2	2:C:533:LEU:O	2.35	0.60
5:L:428:SER:O	5:L:432:THR:OG1	2.17	0.59
3:J:245:LEU:HD23	3:J:250:ARG:HG2	1.83	0.59
3:J:232:ASN:OD1	3:J:232:ASN:N	2.34	0.59
3:D:370:LYS:HB3	3:D:409:TRP:HZ3	1.66	0.59
2:I:1070:HIS:NE2	2:I:1114:GLU:OE2	2.35	0.59
3:D:232:ASN:OD1	3:D:232:ASN:N	2.32	0.59
1:G:71:LYS:NZ	1:G:139:SER:O	2.34	0.59
5:F:354:THR:HG22	5:F:357:GLN:HE21	1.66	0.59
2:C:338:THR:HG21	2:C:345:PRO:HB3	1.84	0.59
5:L:354:THR:H	5:L:357:GLN:HE21	1.48	0.59
2:I:185:ASP:HB2	2:I:197:ARG:HB2	1.84	0.59
3:D:245:LEU:O	3:D:250:ARG:NH1	2.33	0.59
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.29	0.59
3:J:781:LYS:HB3	6:N:5:MEA:CD1	2.31	0.59
2:I:246:LEU:HB3	2:I:269:ILE:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:611:GLU:OE1	2:I:637:ARG:NH1	2.35	0.59
3:D:113:HIS:CD2	3:D:115:TRP:HB2	2.37	0.59
1:A:78:ILE:HD13	1:A:81:ILE:HD12	1.84	0.59
2:I:926:GLY:HA3	2:I:1055:ALA:O	2.02	0.59
1:G:78:ILE:HD13	1:G:81:ILE:HD12	1.84	0.59
1:A:59:VAL:HG21	1:A:85:LEU:HD13	1.85	0.59
3:J:708:ASN:N	3:J:712:GLN:O	2.28	0.59
3:D:746:LEU:CD2	3:D:758:PRO:HB3	2.33	0.58
1:G:66:HIS:HD2	1:G:68:TYR:HB2	1.68	0.58
5:F:151:VAL:HG11	5:F:158:LEU:HG	1.83	0.58
1:H:29:GLU:CG	1:H:30:PRO:HD2	2.30	0.58
4:E:15:ASN:O	4:E:17:PHE:N	2.36	0.58
6:M:5:MEA:C	6:M:7:SER:N	2.65	0.58
1:H:100:LEU:HD21	1:H:121:VAL:HG21	1.84	0.58
2:I:1257:GLN:HG2	2:I:1296:ASP:HB3	1.85	0.58
1:H:133:LEU:HD21	1:H:140:ILE:HG12	1.85	0.58
1:H:71:LYS:NZ	1:H:139:SER:O	2.37	0.58
2:C:246:LEU:HB3	2:C:269:ILE:HD13	1.85	0.58
5:L:422:ARG:HH11	5:L:422:ARG:HG2	1.68	0.58
5:L:435:ILE:O	5:L:439:ILE:HG13	2.04	0.58
2:I:979:LEU:HD21	2:I:1000:LEU:HD23	1.85	0.58
3:J:847:ASP:HA	3:J:860:ARG:HB2	1.85	0.57
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.03	0.57
2:C:975:ILE:HD11	2:C:997:TRP:HE3	1.69	0.57
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.87	0.57
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.84	0.57
2:C:221:LEU:HD12	2:C:313:ALA:HB1	1.86	0.57
1:A:319:GLU:O	1:A:320:ASN:ND2	2.38	0.57
2:C:444:ASP:O	2:C:450:ASN:ND2	2.36	0.57
2:C:979:LEU:HD21	2:C:1000:LEU:HD23	1.85	0.57
5:L:277:MET:HE2	5:L:281:ARG:HG3	1.87	0.57
2:I:150:HIS:CE1	2:I:454:ARG:HD2	2.40	0.57
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.86	0.57
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.86	0.57
2:C:1336:ASN:N	3:D:23:ALA:O	2.36	0.57
3:D:514:THR:HB	3:D:595:ALA:HA	1.87	0.57
5:L:151:VAL:HG11	5:L:158:LEU:HG	1.87	0.57
3:D:781:LYS:HB3	6:M:5:MEA:HD1	1.85	0.57
3:D:775:SER:O	3:D:777:HIS:N	2.38	0.57
1:B:71:LYS:NZ	1:B:139:SER:O	2.38	0.57
3:J:1225:GLY:O	3:J:1229:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:218:ARG:HH11	5:F:218:ARG:CG	2.18	0.56
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.87	0.56
5:F:213:ASP:OD1	5:F:213:ASP:N	2.37	0.56
1:G:230:ALA:O	1:G:232:VAL:N	2.39	0.56
2:C:578:TYR:CD2	2:C:659:GLN:HG2	2.41	0.56
3:J:520:ALA:HB2	3:J:707:ILE:O	2.06	0.56
2:C:1243:MET:O	2:C:1244:HIS:ND1	2.39	0.56
2:I:180:ARG:NH2	2:I:392:GLU:O	2.38	0.56
5:F:262:VAL:HG12	5:F:263:PRO:HD2	1.86	0.56
2:C:1255:THR:HB	2:C:1257:GLN:HG3	1.88	0.56
3:J:102:MET:HG2	3:J:246:PRO:HD3	1.88	0.56
2:C:915:ASP:OD2	2:C:919:ARG:NH2	2.39	0.56
1:G:52:PRO:HG3	1:G:150:ARG:NH1	2.20	0.56
3:J:46:TYR:CZ	3:J:47:ARG:HG3	2.41	0.56
2:C:1340:GLU:HB2	3:D:19:ALA:HB3	1.87	0.56
2:I:1075:VAL:HG21	3:J:354:VAL:HG11	1.86	0.56
2:C:812:PHE:HB3	3:D:357:VAL:HG21	1.88	0.55
3:D:46:TYR:CZ	3:D:47:ARG:HG3	2.41	0.55
5:F:251:LYS:O	5:F:255:VAL:HG23	2.06	0.55
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.88	0.55
2:C:404:LYS:HE2	2:C:586:PHE:CZ	2.41	0.55
3:J:816:THR:HG21	3:J:889:ASP:HB3	1.88	0.55
1:B:25:LYS:HE2	1:B:204:GLU:HG3	1.88	0.55
3:D:879:ALA:O	3:D:880:VAL:HG12	2.07	0.55
2:I:1244:HIS:HB2	2:I:1265:PHE:CG	2.42	0.55
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.34	0.55
3:J:805:GLN:HE21	3:J:1347:LEU:HB2	1.71	0.55
2:I:237:LEU:HD13	2:I:292:ILE:HD12	1.89	0.55
3:J:301:GLU:CD	3:J:312:ARG:HH11	2.10	0.54
2:I:444:ASP:OD1	2:I:447:HIS:N	2.33	0.54
2:C:677:ASN:ND2	2:C:677:ASN:H	2.05	0.54
3:J:556:GLU:O	3:J:558:ASP:N	2.40	0.54
3:J:491:LEU:HA	3:J:499:ILE:H	1.72	0.54
1:G:100:LEU:HD21	1:G:121:VAL:HG21	1.89	0.54
2:C:1070:HIS:NE2	2:C:1114:GLU:OE2	2.39	0.54
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.22	0.54
3:D:298:MET:HG2	5:F:402:LEU:HD23	1.89	0.54
2:I:342:ASP:HA	2:I:437:ASN:HB3	1.89	0.54
5:L:251:LYS:O	5:L:255:VAL:HG23	2.07	0.54
2:C:901:LEU:O	2:C:905:ILE:HG13	2.07	0.54
3:J:114:ILE:HD11	3:J:304:ASP:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:726:TYR:HB2	2:C:733:VAL:HB	1.89	0.54
2:C:103:VAL:HG22	2:C:117:ILE:HG12	1.90	0.54
5:F:250:LEU:O	5:F:254:GLU:HG2	2.07	0.54
1:A:52:PRO:HG3	1:A:150:ARG:NH1	2.22	0.54
1:A:168:ILE:HA	1:B:310:ARG:HA	1.89	0.54
1:B:322:PRO:HB2	1:B:323:PRO:CD	2.38	0.54
2:C:785:ASP:OD2	2:C:791:LEU:N	2.38	0.54
1:B:33:ARG:HB2	1:B:197:ASP:O	2.08	0.54
2:I:728:ASP:HB2	2:I:731:ARG:NH1	2.23	0.54
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.43	0.54
3:D:650:LYS:NZ	3:D:765:GLU:OE2	2.36	0.54
2:C:804:PHE:HE2	2:C:1115:THR:HG21	1.71	0.54
3:J:1329:THR:O	3:J:1333:THR:HG23	2.06	0.54
2:C:150:HIS:CE1	2:C:454:ARG:HD2	2.42	0.54
3:D:738:ARG:NH2	6:M:1:28H:H6	2.23	0.54
2:I:621:SER:HB2	2:I:629:PHE:HE1	1.72	0.54
2:C:868:SER:OG	2:C:944:ARG:HB2	2.08	0.54
3:J:481:ARG:HA	3:J:485:MET:HG2	1.89	0.54
1:G:37:HIS:CE1	1:G:187:VAL:HG21	2.43	0.54
3:D:1225:GLY:HA3	3:J:1295:ASN:O	2.08	0.54
1:G:29:GLU:CB	1:G:30:PRO:HD2	2.38	0.53
3:D:278:ARG:HD3	5:F:406:GLN:HB3	1.89	0.53
2:I:801:ARG:HH21	2:I:1227:VAL:HG11	1.73	0.53
6:N:1:28H:H9	6:N:2:THR:N	2.06	0.53
3:D:1296:GLY:HA3	3:J:1225:GLY:HA2	1.89	0.53
3:D:1295:ASN:O	3:J:1225:GLY:HA3	2.08	0.53
3:D:767:LEU:HD12	3:D:767:LEU:H	1.73	0.53
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.36	0.53
2:C:1289:GLU:HB3	2:C:1294:LYS:HD2	1.90	0.53
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.89	0.53
3:J:297:ARG:NH2	5:L:104:GLU:OE2	2.42	0.53
6:N:5:MEA:O	6:N:7:SER:N	2.42	0.53
2:I:1226:THR:HG21	3:J:639:VAL:O	2.09	0.53
3:D:1221:LEU:HD22	3:D:1306:LEU:HB2	1.90	0.53
5:L:383:ASN:N	5:L:383:ASN:HD22	2.06	0.53
2:C:962:GLU:O	2:C:966:ILE:HG13	2.09	0.53
3:D:739:GLN:NE2	3:D:744:ARG:HG3	2.24	0.53
2:I:404:LYS:HE2	2:I:586:PHE:CZ	2.44	0.53
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.43	0.53
3:J:1216:ALA:HB3	3:J:1219:ASP:HB2	1.89	0.53
1:A:286:GLU:OE1	1:A:304:LYS:NZ	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:5:MEA:O	6:M:7:SER:N	2.42	0.53
3:D:1329:THR:O	3:D:1333:THR:HG23	2.09	0.53
3:D:179:LYS:O	3:D:184:ALA:HB2	2.08	0.53
5:F:277:MET:HE1	5:F:359:LYS:HG2	1.91	0.53
2:C:898:GLU:HG2	5:F:541:ARG:HA	1.89	0.53
2:I:975:ILE:HD11	2:I:997:TRP:HE3	1.73	0.53
2:I:812:PHE:HB3	3:J:357:VAL:HG21	1.91	0.53
2:C:905:ILE:HD11	5:F:598:LEU:HD13	1.91	0.52
5:L:250:LEU:O	5:L:254:GLU:HG2	2.08	0.52
2:I:144:VAL:HG23	2:I:515:MET:SD	2.49	0.52
3:D:145:VAL:HA	3:D:159:ILE:HA	1.90	0.52
3:D:704:GLU:O	3:D:715:LYS:HA	2.09	0.52
5:L:406:GLN:OE1	5:L:406:GLN:HA	2.09	0.52
2:I:1334:GLY:O	3:J:25:ALA:HB3	2.09	0.52
1:B:302:GLU:HB2	2:C:943:LYS:NZ	2.24	0.52
3:D:381:ILE:HA	3:D:415:VAL:HG21	1.91	0.52
2:I:1173:ALA:O	2:I:1177:ARG:N	2.41	0.52
1:B:133:LEU:HD21	1:B:140:ILE:HG12	1.90	0.52
1:A:14:VAL:HG11	1:A:29:GLU:HG2	1.92	0.52
2:I:808:ASN:H	3:J:633:ALA:HB2	1.75	0.52
3:D:1225:GLY:O	3:D:1229:VAL:HG23	2.10	0.52
6:M:5:MEA:O	6:M:6:2TL:C	2.57	0.52
2:I:1087:TYR:CZ	2:I:1213:TYR:HB2	2.45	0.52
3:J:746:LEU:HD22	3:J:758:PRO:HB3	1.92	0.52
3:D:814:CYS:HB3	3:D:890:THR:OG1	2.09	0.52
3:D:746:LEU:O	6:M:2:THR:HG22	2.10	0.51
5:L:218:ARG:HH11	5:L:218:ARG:CG	2.20	0.51
3:J:108:ALA:HB2	3:J:280:LYS:HG3	1.91	0.51
2:C:1192:GLU:OE2	3:D:764:ARG:HD3	2.10	0.51
2:I:798:GLN:OE1	2:I:828:PHE:N	2.43	0.51
1:H:51:MET:CB	1:H:179:PRO:HD2	2.37	0.51
5:F:428:SER:O	5:F:432:THR:OG1	2.27	0.51
2:I:726:TYR:HB2	2:I:733:VAL:HB	1.90	0.51
1:G:44:ARG:HG3	1:G:183:ILE:HB	1.91	0.51
3:D:510:LEU:O	3:D:514:THR:OG1	2.27	0.51
5:L:344:LEU:HD12	5:L:347:ILE:HD12	1.93	0.51
2:C:1199:LEU:O	2:C:1204:LEU:N	2.40	0.51
3:D:275:ARG:NH2	5:F:400:GLN:OE1	2.43	0.51
6:N:5:MEA:O	6:N:6:2TL:C	2.57	0.51
1:A:319:GLU:C	1:A:320:ASN:HD22	2.14	0.51
5:L:363:ARG:O	5:L:367:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:GLU:O	1:G:218:ARG:HG3	2.10	0.51
1:A:285:THR:HG23	1:A:288:GLU:H	1.76	0.51
1:A:68:TYR:CE2	2:C:831:ILE:HD11	2.46	0.51
2:I:344:GLY:H	2:I:437:ASN:ND2	2.08	0.51
3:J:301:GLU:OE1	5:L:97:PRO:HG3	2.09	0.51
5:F:134:VAL:HG11	5:F:266:PHE:CE1	2.44	0.51
5:L:383:ASN:O	5:L:386:LEU:N	2.39	0.51
2:C:48:GLY:O	2:C:50:GLU:N	2.37	0.51
3:D:1257:VAL:HA	3:D:1260:MET:HE3	1.91	0.51
5:L:226:ALA:HA	5:L:229:VAL:HG22	1.93	0.51
5:L:145:LEU:HD12	5:L:228:TYR:HD2	1.74	0.51
1:A:44:ARG:NH1	2:C:1087:TYR:OH	2.43	0.51
3:J:56:LEU:HB3	3:J:250:ARG:NH2	2.25	0.51
5:F:292:VAL:HA	5:F:297:MET:O	2.10	0.51
3:D:245:LEU:HD23	3:D:250:ARG:HG2	1.93	0.50
1:B:7:GLU:O	1:B:8:PHE:HB2	2.10	0.50
5:L:585:GLU:OE1	5:L:588:ARG:NH2	2.44	0.50
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.45	0.50
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.92	0.50
5:L:231:THR:HA	5:L:234:THR:HG23	1.92	0.50
3:J:879:ALA:O	3:J:880:VAL:HG12	2.11	0.50
5:F:383:ASN:HD22	5:F:383:ASN:N	2.09	0.50
3:D:746:LEU:N	3:D:746:LEU:CD2	2.74	0.50
5:F:261:LEU:HB2	5:F:266:PHE:CE2	2.46	0.50
2:C:890:LYS:HD3	2:C:914:LYS:HE3	1.93	0.50
1:A:29:GLU:CB	1:A:30:PRO:HD2	2.41	0.50
5:L:397:ARG:HB3	5:L:443:ILE:HD13	1.94	0.50
3:J:842:ARG:NH2	3:J:1254:GLU:OE1	2.44	0.50
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.93	0.50
1:B:286:GLU:OE1	1:B:304:LYS:NZ	2.35	0.50
2:I:909:LYS:O	2:I:911:SER:N	2.44	0.50
1:G:152:TYR:HD2	2:I:824:GLN:CG	2.25	0.50
3:J:615:LYS:H	4:K:7:GLN:CG	2.24	0.50
3:D:317:THR:HB	3:D:319:SER:O	2.11	0.50
3:D:747:MET:HA	6:M:2:THR:HG21	1.93	0.50
2:I:225:PHE:HE1	2:I:345:PRO:HA	1.77	0.50
2:I:1255:THR:HB	2:I:1257:GLN:HG3	1.92	0.50
2:I:801:ARG:HE	2:I:1227:VAL:CG1	2.25	0.50
5:L:292:VAL:HA	5:L:297:MET:O	2.11	0.50
3:D:775:SER:O	3:D:778:GLY:N	2.43	0.50
2:C:404:LYS:HE2	2:C:586:PHE:HZ	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.46	0.50
5:F:551:LEU:HB2	5:F:555:GLU:HG3	1.92	0.50
2:I:1333:LEU:HD13	3:J:115:TRP:CZ3	2.47	0.50
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.12	0.50
3:J:647:PRO:HG3	3:J:697:MET:HA	1.93	0.50
2:I:703:GLY:N	2:I:705:GLU:OE2	2.44	0.50
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.77	0.50
1:B:182:ARG:HD3	3:D:531:LYS:CA	2.37	0.50
3:J:370:LYS:HB3	3:J:409:TRP:HZ3	1.75	0.50
2:C:150:HIS:CD2	2:C:152:SER:HG	2.29	0.50
1:A:107:ILE:HG13	1:A:136:GLU:HG3	1.94	0.50
5:L:469:GLN:O	5:L:473:GLU:HG2	2.12	0.50
1:H:41:ASN:ND2	2:I:1217:THR:HG22	2.27	0.50
3:J:739:GLN:NE2	3:J:744:ARG:HG3	2.25	0.49
3:D:317:THR:HG22	3:D:323:PRO:HA	1.94	0.49
3:J:597:GLY:H	3:J:600:ALA:HB3	1.77	0.49
1:B:285:THR:HG23	1:B:288:GLU:H	1.77	0.49
2:C:728:ASP:HB2	2:C:731:ARG:NH1	2.27	0.49
2:C:1226:THR:HG23	3:D:638:SER:OG	2.11	0.49
3:J:1244:GLN:OE1	3:J:1244:GLN:HA	2.12	0.49
5:F:276:MET:SD	5:F:279:ARG:NH2	2.85	0.49
5:F:299:LYS:O	5:F:303:ILE:HG12	2.13	0.49
2:C:703:GLY:N	2:C:705:GLU:OE2	2.46	0.49
2:C:151:ARG:NH2	2:C:445:ILE:HD13	2.27	0.49
5:L:231:THR:O	5:L:235:ILE:HG12	2.12	0.49
1:B:78:ILE:HD13	1:B:81:ILE:HD12	1.94	0.49
1:H:66:HIS:HD2	1:H:68:TYR:HB3	1.77	0.49
3:J:738:ARG:NH2	6:N:1:28H:H6	2.24	0.49
2:C:1253:LEU:HA	5:F:525:ASP:HB2	1.93	0.49
5:L:306:PHE:O	5:L:308:GLY:N	2.44	0.49
3:J:382:TYR:HB3	3:J:394:ILE:HG23	1.95	0.49
3:D:382:TYR:HB3	3:D:394:ILE:HG23	1.94	0.49
2:C:736:VAL:O	2:C:737:ASN:HB2	2.13	0.49
3:D:435:GLN:HB2	3:D:457:TYR:OH	2.13	0.49
3:D:647:PRO:HG3	3:D:697:MET:HA	1.95	0.49
2:I:40:GLU:O	2:I:73:TYR:OH	2.27	0.49
3:D:686:TRP:HB3	3:D:746:LEU:HD21	1.95	0.49
5:L:590:ILE:HA	5:L:593:LYS:HG2	1.95	0.49
1:B:301:THR:HG22	2:C:867:GLU:OE2	2.12	0.49
1:B:302:GLU:HB2	2:C:943:LYS:HZ2	1.78	0.49
1:A:29:GLU:CG	1:A:30:PRO:HD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:27:ALA:HB2	4:K:47:THR:HA	1.95	0.49
2:I:804:PHE:HE2	2:I:1115:THR:HG21	1.76	0.49
3:J:145:VAL:O	3:J:178:ALA:HA	2.13	0.49
1:H:42:ALA:O	1:H:46:ILE:HG12	2.13	0.49
2:C:1268:GLN:HE22	3:D:352:ARG:HB3	1.77	0.49
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.47	0.49
3:D:767:LEU:HD11	3:D:772:TYR:HD2	1.78	0.49
1:A:42:ALA:O	1:A:46:ILE:HG12	2.13	0.49
1:H:180:VAL:HG11	1:H:183:ILE:HD11	1.95	0.49
1:B:17:GLU:HB3	1:B:25:LYS:HB2	1.94	0.49
2:C:103:VAL:HG12	2:C:104:ILE:O	2.13	0.49
2:C:1209:GLN:HA	2:C:1226:THR:HA	1.95	0.48
2:I:756:TYR:H	2:I:766:ASN:HB3	1.77	0.48
2:C:542:ARG:NH2	2:C:542:ARG:HG2	2.27	0.48
2:I:27:LEU:HD23	2:I:711:ASP:OD2	2.14	0.48
5:F:437:GLN:HG3	5:F:438:ALA:N	2.28	0.48
5:L:299:LYS:O	5:L:303:ILE:HG12	2.13	0.48
1:G:29:GLU:CG	1:G:30:PRO:HD2	2.43	0.48
3:J:1257:VAL:HA	3:J:1260:MET:HE3	1.95	0.48
1:G:134:THR:OG1	1:G:135:ASP:N	2.46	0.48
1:H:86:LYS:HG2	1:H:173:VAL:CG2	2.42	0.48
2:I:150:HIS:CE1	2:I:152:SER:HA	2.48	0.48
5:L:394:TYR:OH	5:L:436:ARG:HG3	2.13	0.48
6:M:1:28H:H9	6:M:2:THR:N	2.11	0.48
2:C:694:ARG:HH11	2:C:694:ARG:CG	2.26	0.48
5:L:383:ASN:H	5:L:383:ASN:HD22	1.62	0.48
3:J:550:VAL:O	3:J:569:LEU:HA	2.14	0.48
1:H:102:LEU:HG	1:H:115:ILE:HG12	1.96	0.48
5:L:344:LEU:HG	5:L:355:ILE:HD12	1.94	0.48
1:B:42:ALA:O	1:B:46:ILE:HG12	2.14	0.48
5:F:231:THR:O	5:F:235:ILE:HG12	2.13	0.48
5:F:226:ALA:HA	5:F:229:VAL:HG22	1.95	0.48
1:H:14:VAL:HG11	1:H:29:GLU:CD	2.33	0.48
2:C:796:LEU:H	2:C:1231:TYR:HH	1.59	0.48
3:D:550:VAL:O	3:D:569:LEU:HA	2.14	0.48
5:L:324:LYS:HB3	5:L:325:PRO:HD2	1.95	0.48
2:I:930:ASP:HB2	2:I:1053:TYR:HB2	1.95	0.48
2:C:542:ARG:CG	2:C:542:ARG:HH21	2.27	0.48
3:J:410:ASP:O	3:J:414:GLU:HG3	2.13	0.48
3:D:507:VAL:HG21	3:D:598:LYS:HB2	1.96	0.48
5:F:216:LEU:O	5:F:219:GLU:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:98:VAL:HG22	5:L:402:LEU:HD13	1.95	0.48
5:L:383:ASN:N	5:L:383:ASN:ND2	2.62	0.48
3:J:113:HIS:HB3	3:J:116:PHE:HD2	1.79	0.48
3:D:1146:GLU:OE2	3:D:1310:THR:OG1	2.32	0.48
2:C:14:ASP:HB3	2:C:1158:LYS:CB	2.44	0.48
2:C:890:LYS:HE3	2:C:911:SER:O	2.14	0.47
5:F:324:LYS:HB3	5:F:325:PRO:HD2	1.95	0.47
2:C:145:ILE:HB	2:C:456:VAL:HG13	1.95	0.47
2:I:225:PHE:CE1	2:I:345:PRO:HA	2.49	0.47
3:J:260:PHE:HB3	5:L:504:PRO:HB3	1.96	0.47
2:C:560:PRO:HB2	3:D:776:THR:CB	2.44	0.47
5:F:355:ILE:HG13	5:F:355:ILE:H	1.41	0.47
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.45	0.47
1:B:95:LYS:HE2	1:B:95:LYS:HA	1.96	0.47
3:J:745:GLY:CA	6:N:1:28H:H11	2.35	0.47
5:F:433:TRP:O	5:F:437:GLN:HB3	2.15	0.47
5:F:407:GLU:HG3	5:F:442:SER:OG	2.14	0.47
3:J:1163:VAL:N	3:J:1202:GLU:O	2.47	0.47
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.97	0.47
3:J:821:MET:HA	3:J:881:LYS:HA	1.96	0.47
2:I:25:PRO:HD3	2:I:578:TYR:CD1	2.48	0.47
3:J:1161:GLY:O	3:J:1204:VAL:N	2.48	0.47
2:I:1239:VAL:HG13	3:J:354:VAL:HB	1.97	0.47
2:C:801:ARG:HE	2:C:1227:VAL:HG11	1.79	0.47
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.14	0.47
3:J:733:SER:O	3:J:737:ILE:HG12	2.14	0.47
1:B:107:ILE:HG13	1:B:136:GLU:HG3	1.96	0.47
1:H:95:LYS:HA	1:H:95:LYS:HE2	1.97	0.47
6:M:4:D4P:HA	6:M:5:MEA:HC1	1.57	0.47
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.29	0.47
3:J:553:THR:HA	3:J:567:THR:HA	1.95	0.47
3:J:865:HIS:O	3:J:869:CYS:N	2.36	0.47
1:G:42:ALA:O	1:G:46:ILE:HG12	2.15	0.47
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.45	0.47
2:I:1222:GLU:OE2	3:J:512:TYR:OH	2.24	0.47
1:H:155:ALA:HB1	1:H:172:LEU:HB2	1.96	0.47
1:H:30:PRO:HB3	1:H:198:LEU:HD13	1.96	0.47
1:H:82:LEU:HD21	1:H:171:LEU:HD12	1.96	0.47
2:C:867:GLU:HG2	2:C:943:LYS:HZ3	1.80	0.47
3:D:108:ALA:HB2	3:D:280:LYS:HG3	1.96	0.47
2:I:944:ARG:HH21	2:I:1050:VAL:HG13	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:124:GLU:CD	5:L:422:ARG:HH12	2.16	0.47
3:J:893:GLY:O	3:J:1258:ARG:NH2	2.38	0.47
3:J:894:VAL:HG13	3:J:895:CYS:N	2.30	0.47
3:D:894:VAL:HG13	3:D:895:CYS:N	2.30	0.47
5:F:306:PHE:O	5:F:308:GLY:N	2.48	0.47
5:F:590:ILE:HA	5:F:593:LYS:HG2	1.96	0.47
3:D:1244:GLN:OE1	3:D:1244:GLN:HA	2.14	0.47
1:H:212:ASP:HB2	1:H:215:GLU:HG2	1.97	0.47
5:F:383:ASN:ND2	5:F:383:ASN:N	2.62	0.47
5:F:520:GLY:HA2	5:F:523:ILE:HD12	1.97	0.47
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.96	0.47
1:G:95:LYS:HA	1:G:95:LYS:HE2	1.97	0.47
5:L:387:VAL:HG23	5:L:412:LEU:HD22	1.97	0.46
1:A:30:PRO:HB3	1:A:198:LEU:HD13	1.97	0.46
2:C:1314:GLN:HB2	3:D:473:THR:CB	2.45	0.46
5:F:363:ARG:O	5:F:367:ILE:HG13	2.15	0.46
3:J:857:LEU:HA	3:J:858:VAL:HA	1.70	0.46
2:I:716:ALA:HB3	2:I:784:ALA:HB3	1.96	0.46
1:A:95:LYS:HA	1:A:95:LYS:HE2	1.97	0.46
3:D:271:ARG:NH1	5:F:400:GLN:OE1	2.48	0.46
3:J:930:LEU:O	3:J:931:THR:HB	2.16	0.46
1:A:38:THR:HG23	1:B:42:ALA:HA	1.97	0.46
3:J:834:PRO:O	3:J:835:LEU:HB2	2.15	0.46
3:D:410:ASP:O	3:D:414:GLU:HG3	2.15	0.46
3:J:510:LEU:O	3:J:514:THR:OG1	2.33	0.46
1:B:56:VAL:HG12	1:B:173:VAL:HG11	1.96	0.46
2:I:1297:ASP:OD1	2:I:1300:GLY:N	2.23	0.46
5:F:97:PRO:HB2	5:F:402:LEU:HD21	1.96	0.46
3:D:210:SER:O	3:D:214:ARG:NH2	2.47	0.46
5:F:132:CYS:O	5:F:136:GLU:HG3	2.15	0.46
1:B:52:PRO:HG3	1:B:150:ARG:HH12	1.80	0.46
1:A:152:TYR:CE2	2:C:824:GLN:HA	2.50	0.46
1:B:260:LEU:HD23	1:B:310:ARG:HH11	1.80	0.46
1:B:321:TRP:CE3	1:B:321:TRP:HA	2.51	0.46
3:D:546:ALA:O	3:D:573:THR:HA	2.15	0.46
3:D:491:LEU:HD21	3:D:609:TYR:CZ	2.50	0.46
2:I:1259:LEU:HD12	2:I:1260:GLY:N	2.30	0.46
3:J:298:MET:HG2	5:L:402:LEU:HD23	1.96	0.46
1:G:107:ILE:HG13	1:G:136:GLU:HG3	1.97	0.46
2:C:903:ARG:NH1	2:C:908:GLU:OE1	2.36	0.46
3:D:297:ARG:HG2	5:F:97:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:650:LYS:HE3	3:J:743:MET:HB2	1.98	0.46
1:H:107:ILE:HG13	1:H:136:GLU:HG3	1.97	0.46
1:A:102:LEU:HG	1:A:115:ILE:HG12	1.97	0.46
5:L:277:MET:CE	5:L:359:LYS:HG2	2.45	0.46
2:C:867:GLU:N	2:C:867:GLU:OE1	2.48	0.46
2:C:645:PHE:CG	2:C:649:GLN:HB2	2.51	0.46
5:L:557:LYS:HB3	5:L:580:PHE:HZ	1.81	0.46
2:I:905:ILE:HD11	5:L:598:LEU:HD13	1.98	0.46
1:A:143:ARG:HD2	1:A:143:ARG:N	2.31	0.46
3:D:816:THR:HG21	3:D:889:ASP:HB3	1.97	0.46
5:F:383:ASN:H	5:F:383:ASN:HD22	1.64	0.46
1:A:134:THR:HG21	2:C:727:VAL:O	2.16	0.46
5:L:437:GLN:HG3	5:L:438:ALA:N	2.30	0.46
3:D:141:PHE:CD2	3:D:293:ARG:HG3	2.50	0.46
3:D:901:ARG:O	3:D:1251:LYS:NZ	2.49	0.46
2:C:539:THR:O	2:C:540:ARG:HB2	2.16	0.46
5:L:134:VAL:HG11	5:L:266:PHE:HE1	1.81	0.46
3:D:746:LEU:N	6:M:1:28H:H11	2.31	0.46
3:D:127:LEU:HD11	3:D:227:PHE:CE2	2.51	0.46
5:L:420:GLU:O	5:L:423:ARG:HB2	2.15	0.46
2:C:890:LYS:O	2:C:892:GLU:HG3	2.16	0.46
2:I:1328:LYS:HD3	2:I:1328:LYS:HA	1.80	0.46
3:J:842:ARG:HD2	3:J:842:ARG:HA	1.57	0.45
1:A:62:ASP:OD2	1:A:143:ARG:NH2	2.49	0.45
3:D:1172:LYS:HA	3:D:1192:LYS:H	1.81	0.45
1:G:76:GLU:HB2	1:G:80:GLU:HB2	1.97	0.45
6:M:5:MEA:C	6:M:7:SER:H	2.29	0.45
3:J:686:TRP:CD2	3:J:758:PRO:HG3	2.51	0.45
1:A:46:ILE:HG21	1:A:220:ALA:HA	1.98	0.45
2:I:887:VAL:HB	2:I:913:VAL:HB	1.99	0.45
2:C:1150:ASP:HA	2:C:1153:ALA:HB3	1.97	0.45
1:G:86:LYS:NZ	2:I:826:ASP:OD2	2.49	0.45
1:A:321:TRP:HA	1:A:321:TRP:CE3	2.51	0.45
2:I:745:GLU:HA	2:I:1014:LEU:HD21	1.97	0.45
2:C:474:ALA:HB1	2:C:478:ARG:NH2	2.31	0.45
1:A:42:ALA:HA	1:B:38:THR:HG23	1.98	0.45
3:D:730:ALA:O	3:D:731:ARG:HG2	2.16	0.45
3:D:660:GLU:O	3:D:664:ILE:HG13	2.15	0.45
2:C:85:CYS:HB3	2:C:90:VAL:O	2.17	0.45
5:L:584:ARG:O	5:L:587:ILE:HG22	2.16	0.45
3:J:374:LEU:O	3:J:378:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:265:LEU:HD23	3:D:268:LEU:HD12	1.98	0.45
1:H:41:ASN:HD21	2:I:1217:THR:HG22	1.80	0.45
2:I:67:GLU:N	2:I:103:VAL:O	2.29	0.45
2:I:85:CYS:HB3	2:I:90:VAL:O	2.15	0.45
5:L:117:ILE:O	5:L:121:LYS:HG3	2.15	0.45
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.98	0.45
6:N:1:28H:CBX	6:N:1:28H:H6	2.46	0.45
3:D:744:ARG:HE	6:M:2:THR:HA	1.82	0.45
5:F:225:ARG:O	5:F:229:VAL:HG13	2.16	0.45
2:I:933:VAL:HG13	2:I:1050:VAL:HG22	1.99	0.45
1:A:322:PRO:HB2	1:A:323:PRO:CD	2.46	0.45
5:F:344:LEU:HD12	5:F:347:ILE:HD12	1.98	0.45
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.51	0.45
2:I:1087:TYR:CE2	2:I:1213:TYR:HB2	2.51	0.45
3:D:504:GLN:HB2	3:D:505:ASP:H	1.56	0.45
1:G:51:MET:HA	1:G:52:PRO:HD3	1.62	0.45
3:D:733:SER:O	3:D:737:ILE:HG12	2.17	0.45
2:I:785:ASP:OD2	2:I:791:LEU:N	2.45	0.45
3:J:435:GLN:HB2	3:J:457:TYR:OH	2.16	0.45
2:C:682:GLY:O	2:C:686:GLN:HG3	2.17	0.45
5:F:277:MET:HE2	5:F:281:ARG:HG3	1.99	0.45
1:H:180:VAL:HA	1:H:207:THR:HA	1.98	0.45
2:I:562:GLU:OE1	2:I:662:SER:OG	2.21	0.45
2:I:338:THR:HG21	2:I:345:PRO:HB3	2.00	0.44
3:D:930:LEU:O	3:D:931:THR:HB	2.16	0.44
3:D:762:ASN:O	3:D:765:GLU:N	2.50	0.44
2:I:142:GLU:O	2:I:515:MET:HB2	2.17	0.44
3:D:609:TYR:HA	3:D:617:THR:OG1	2.16	0.44
2:I:52:ALA:O	2:I:56:VAL:HG23	2.17	0.44
3:J:425:ARG:HB2	3:J:466:MET:HG2	1.98	0.44
2:I:1212:LEU:HB3	2:I:1221:PHE:HD2	1.81	0.44
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.48	0.44
1:B:195:ARG:O	1:B:196:THR:HG22	2.17	0.44
2:I:539:THR:O	2:I:540:ARG:HB2	2.16	0.44
6:N:5:MEA:C	6:N:7:SER:H	2.29	0.44
6:M:2:THR:CG2	6:M:6:2TL:O	2.63	0.44
1:A:51:MET:HA	1:A:52:PRO:HD3	1.67	0.44
2:I:801:ARG:HE	2:I:1227:VAL:HG11	1.82	0.44
2:I:844:LYS:HE3	3:J:49:PHE:CZ	2.51	0.44
2:I:84:GLU:OE2	2:I:1035:LYS:HD2	2.17	0.44
2:I:15:PHE:HE2	2:I:1198:LEU:HD11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:775:SER:O	3:D:776:THR:C	2.56	0.44
5:F:148:TYR:C	5:F:150:ARG:H	2.21	0.44
2:I:101:ARG:HB2	2:I:117:ILE:HD12	1.99	0.44
2:C:756:TYR:H	2:C:766:ASN:HB3	1.82	0.44
1:A:279:GLY:O	1:A:283:GLN:HG3	2.18	0.44
2:I:1077:SER:HA	3:J:356:THR:HB	1.99	0.44
3:J:781:LYS:HB3	6:N:5:MEA:HD1	1.99	0.44
5:L:559:LEU:HG	5:L:563:PHE:HE2	1.83	0.44
4:E:79:GLU:O	4:E:82:ALA:N	2.50	0.44
5:F:117:ILE:O	5:F:121:LYS:HG3	2.17	0.44
5:L:509:THR:HA	5:L:510:PRO:HD3	1.87	0.44
6:M:2:THR:HG23	6:M:6:2TL:OG1	2.17	0.44
1:H:51:MET:HA	1:H:52:PRO:HD3	1.78	0.44
1:A:22:THR:HB	1:A:207:THR:O	2.17	0.44
5:L:407:GLU:HG3	5:L:442:SER:OG	2.17	0.44
3:D:1164:SER:N	3:D:1178:THR:O	2.39	0.44
3:D:502:PRO:HB3	3:D:506:VAL:HG11	2.00	0.44
1:H:124:VAL:HG21	1:H:210:THR:HB	2.00	0.44
3:J:288:PRO:HG3	5:L:377:LYS:HG3	1.99	0.44
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.53	0.44
1:G:68:TYR:CG	2:I:929:ILE:HG21	2.53	0.44
1:B:321:TRP:HA	1:B:322:PRO:HA	1.69	0.44
2:I:1226:THR:HG23	3:J:638:SER:OG	2.17	0.44
2:C:48:GLY:C	2:C:50:GLU:H	2.18	0.44
5:L:261:LEU:HB2	5:L:266:PHE:CE2	2.53	0.44
2:C:930:ASP:HB2	2:C:1053:TYR:HB2	2.00	0.44
3:D:650:LYS:HE3	3:D:743:MET:HB2	1.99	0.44
2:C:960:LEU:HD22	2:C:1029:LEU:HD12	2.00	0.44
2:I:176:ILE:HD12	2:I:184:LEU:HD23	2.00	0.44
5:F:137:TYR:O	5:F:141:ILE:HG12	2.18	0.44
3:J:179:LYS:HB2	3:J:184:ALA:HB2	2.00	0.44
5:L:145:LEU:HB3	5:L:225:ARG:HH21	1.82	0.44
2:I:1330:ILE:O	2:I:1333:LEU:HB2	2.18	0.44
5:L:433:TRP:O	5:L:437:GLN:HB3	2.17	0.44
5:F:137:TYR:HE2	5:F:273:MET:HB3	1.82	0.44
3:J:730:ALA:O	3:J:731:ARG:HG2	2.17	0.44
1:B:124:VAL:HG21	1:B:210:THR:HG22	2.00	0.44
3:J:787:ALA:O	3:J:790:THR:HG23	2.17	0.44
2:I:1243:MET:SD	3:J:445:LYS:HB3	2.57	0.44
5:L:132:CYS:O	5:L:136:GLU:HG3	2.18	0.44
3:D:746:LEU:O	6:M:1:28H:H12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:936:ARG:NH2	2:C:936:ARG:HG3	2.06	0.44
5:L:354:THR:HG22	5:L:357:GLN:NE2	2.31	0.44
2:C:901:LEU:HD13	5:F:563:PHE:CE2	2.53	0.44
1:H:76:GLU:HB2	1:H:80:GLU:HB2	2.00	0.44
1:A:82:LEU:O	1:A:86:LYS:HG3	2.18	0.44
1:A:287:VAL:O	1:A:291:LYS:HG3	2.17	0.43
2:C:903:ARG:O	2:C:907:GLY:N	2.52	0.43
1:B:82:LEU:O	1:B:86:LYS:HG3	2.18	0.43
3:D:481:ARG:HA	3:D:485:MET:HG2	2.00	0.43
3:J:212:THR:O	3:J:216:LYS:HG2	2.18	0.43
1:H:152:TYR:CD1	1:H:176:CYS:HA	2.52	0.43
2:I:677:ASN:H	2:I:677:ASN:HD22	1.66	0.43
6:N:2:THR:HG23	6:N:6:2TL:OG1	2.17	0.43
1:A:143:ARG:HE	1:B:254:LEU:HD11	1.82	0.43
5:F:420:GLU:O	5:F:423:ARG:HB2	2.18	0.43
3:J:932:MET:HE3	3:J:1138:LEU:HD23	1.99	0.43
3:J:189:LEU:HD12	3:J:238:ILE:HD13	2.00	0.43
2:C:890:LYS:HE2	2:C:914:LYS:HG3	1.99	0.43
3:D:232:ASN:ND2	3:D:1337:VAL:O	2.51	0.43
2:I:221:LEU:HD22	2:I:336:LEU:HD11	2.01	0.43
2:C:155:VAL:HG12	2:C:405:PHE:HA	2.00	0.43
1:B:180:VAL:HG11	1:B:183:ILE:HD11	2.00	0.43
3:D:781:LYS:CB	6:M:5:MEA:HD1	2.48	0.43
1:H:82:LEU:O	1:H:86:LYS:HG3	2.18	0.43
5:L:137:TYR:O	5:L:141:ILE:HG12	2.18	0.43
6:M:1:28H:H6	6:M:1:28H:CBX	2.46	0.43
2:I:392:GLU:HA	2:I:395:TYR:O	2.19	0.43
3:D:109:SER:OG	3:D:296:LYS:HE2	2.17	0.43
5:F:440:THR:HA	5:F:443:ILE:HD11	2.00	0.43
1:B:51:MET:HB3	1:B:179:PRO:HD2	1.99	0.43
5:L:148:TYR:C	5:L:150:ARG:H	2.22	0.43
1:G:41:ASN:ND2	1:G:44:ARG:NH2	2.67	0.43
5:L:344:LEU:HA	5:L:344:LEU:HD12	1.86	0.43
3:D:554:GLU:HA	3:D:580:TRP:CZ2	2.53	0.43
3:D:646:ILE:HG12	3:D:741:ALA:O	2.18	0.43
1:B:279:GLY:O	1:B:283:GLN:HG3	2.19	0.43
1:G:68:TYR:CZ	2:I:1055:ALA:HB1	2.54	0.43
1:G:74:VAL:HG11	1:G:81:ILE:HD11	1.99	0.43
3:J:109:SER:OG	3:J:296:LYS:HE2	2.19	0.43
1:B:273:GLU:OE2	1:B:293:PRO:HD2	2.19	0.43
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:763:PHE:HA	3:D:763:PHE:HD1	1.71	0.43
2:C:870:ILE:HG21	2:C:944:ARG:NH2	2.34	0.43
3:J:762:ASN:O	3:J:765:GLU:N	2.51	0.43
5:L:134:VAL:HA	5:L:273:MET:HE1	2.01	0.43
2:C:478:ARG:HE	2:C:478:ARG:HB2	1.62	0.43
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.35	0.43
5:L:499:LYS:O	5:L:501:ALA:N	2.51	0.43
2:I:1214:ASP:OD2	2:I:1216:ARG:NH1	2.52	0.43
1:B:27:THR:HG22	1:B:202:VAL:HG13	2.00	0.43
1:A:319:GLU:O	1:A:319:GLU:HG3	2.18	0.43
3:J:492:SER:HA	3:J:493:PRO:HD3	1.84	0.43
3:J:899:TYR:CZ	3:J:1251:LYS:HD2	2.54	0.43
3:J:188:LEU:O	3:J:192:MET:HB3	2.19	0.43
3:D:865:HIS:HB3	3:D:868:TRP:CD1	2.48	0.43
5:F:270:VAL:HA	5:F:273:MET:HG3	2.00	0.43
5:L:253:SER:O	5:L:257:LYS:HG3	2.19	0.43
3:D:678:ARG:NH2	3:D:756:GLU:OE1	2.51	0.43
1:A:56:VAL:HG12	1:A:173:VAL:HG11	1.99	0.43
2:I:906:PHE:HB3	2:I:907:GLY:H	1.54	0.43
3:D:893:GLY:C	3:D:1258:ARG:HH12	2.23	0.43
5:F:509:THR:HA	5:F:510:PRO:HD3	1.89	0.43
2:C:590:PRO:HG2	2:C:659:GLN:NE2	2.34	0.42
2:I:844:LYS:HE3	3:J:49:PHE:CE2	2.54	0.42
1:H:52:PRO:HG3	1:H:150:ARG:NH1	2.34	0.42
1:H:47:LEU:HA	1:H:51:MET:HG2	1.99	0.42
1:B:214:GLU:O	1:B:218:ARG:HG3	2.20	0.42
2:I:957:LYS:HA	2:I:1029:LEU:HD11	2.01	0.42
2:C:213:LEU:HD13	2:C:422:LYS:HB2	2.01	0.42
2:I:160:ASP:C	2:I:162:GLY:H	2.23	0.42
1:G:28:LEU:HD12	1:G:201:LEU:HD23	2.01	0.42
3:D:301:GLU:CD	3:D:312:ARG:HH11	2.19	0.42
5:F:101:TYR:CE2	5:F:405:ILE:HD13	2.54	0.42
1:H:211:ILE:HD12	1:H:215:GLU:HG3	2.01	0.42
3:D:761:ALA:HB3	3:D:767:LEU:HB3	2.01	0.42
5:L:402:LEU:HD12	5:L:402:LEU:HA	1.84	0.42
3:J:514:THR:O	3:J:595:ALA:HA	2.19	0.42
5:L:259:PHE:O	5:L:261:LEU:HD12	2.19	0.42
1:A:224:LEU:HD23	1:B:228:LEU:HD11	2.01	0.42
4:E:39:VAL:HA	4:E:40:PRO:CB	2.49	0.42
3:D:69:GLU:HG3	3:D:76:LYS:HG2	2.00	0.42
5:L:296:LYS:HA	5:L:296:LYS:HD3	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:612:LEU:HD22	3:D:612:LEU:O	2.18	0.42
1:H:29:GLU:CB	1:H:30:PRO:HD2	2.48	0.42
2:I:890:LYS:HG2	2:I:914:LYS:HE3	2.00	0.42
1:B:322:PRO:HB2	1:B:323:PRO:HD3	2.01	0.42
5:L:383:ASN:O	5:L:385:ARG:N	2.52	0.42
5:L:598:LEU:HA	5:L:598:LEU:HD23	1.93	0.42
2:C:180:ARG:NH2	2:C:392:GLU:O	2.52	0.42
3:J:836:ARG:O	3:J:840:LEU:N	2.49	0.42
2:C:972:PHE:HB3	2:C:994:ARG:HH21	1.83	0.42
1:B:263:THR:HG22	2:C:947:GLU:HG2	2.00	0.42
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.19	0.42
5:F:300:LYS:HB3	5:F:300:LYS:HE3	1.80	0.42
6:N:1:28H:H10	6:N:1:28H:H3	1.81	0.42
2:I:1099:ASN:HD21	3:J:505:ASP:CG	2.21	0.42
1:H:74:VAL:HG11	1:H:81:ILE:HD11	2.02	0.42
3:D:113:HIS:CD2	3:D:115:TRP:H	2.37	0.42
3:D:506:VAL:HG13	3:D:628:GLY:HA3	2.01	0.42
5:F:397:ARG:HH12	5:F:461:ASN:ND2	2.17	0.42
3:J:814:CYS:HB3	3:J:890:THR:OG1	2.19	0.42
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	2.01	0.42
3:J:50:LYS:HD3	3:J:50:LYS:HA	1.84	0.42
3:J:744:ARG:HE	6:N:2:THR:HA	1.84	0.42
2:I:933:VAL:HG11	2:I:944:ARG:HG3	2.00	0.42
5:L:121:LYS:HE2	5:L:421:TYR:OH	2.20	0.42
2:C:714:VAL:O	2:C:767:GLN:NE2	2.46	0.42
1:B:9:LEU:HA	1:B:9:LEU:HD23	1.81	0.42
3:D:16:GLU:O	3:D:16:GLU:HG2	2.20	0.42
3:D:1272:SER:HB3	3:D:1292:LEU:HD11	2.00	0.42
2:I:1336:ASN:HB2	3:J:25:ALA:HB2	2.02	0.42
3:J:749:LYS:HB2	3:J:753:SER:O	2.20	0.42
3:J:660:GLU:O	3:J:664:ILE:HG13	2.20	0.42
1:A:190:ALA:H	1:A:199:ASP:HA	1.85	0.42
3:D:787:ALA:O	3:D:790:THR:HG23	2.20	0.42
3:D:452:LEU:HG	3:D:625:MET:HE3	2.01	0.42
6:N:2:THR:CG2	6:N:6:2TL:O	2.63	0.42
5:F:97:PRO:HB2	5:F:402:LEU:CD2	2.50	0.42
2:I:346:TYR:O	2:I:350:THR:N	2.49	0.42
2:C:152:SER:OG	2:C:452:ARG:HG2	2.19	0.42
2:C:728:ASP:HB3	2:C:731:ARG:H	1.84	0.42
3:J:796:LEU:HD22	3:J:1138:LEU:HD11	2.01	0.42
2:I:589:THR:OG1	2:I:659:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1328:LYS:HA	2:C:1328:LYS:HD3	1.82	0.42
1:B:10:LYS:CB	1:B:11:PRO:HD2	2.35	0.42
5:F:584:ARG:O	5:F:587:ILE:HG22	2.20	0.42
2:I:227:LYS:NZ	2:I:334:GLU:OE2	2.53	0.42
2:C:890:LYS:HG2	2:C:914:LYS:CG	2.49	0.42
2:C:677:ASN:ND2	2:C:677:ASN:N	2.68	0.42
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.39	0.42
2:C:367:TYR:CD1	2:C:376:PRO:HB3	2.55	0.42
5:L:409:ASN:O	5:L:413:MET:HG3	2.20	0.42
3:J:597:GLY:O	3:J:601:ILE:N	2.44	0.42
3:J:930:LEU:HA	3:J:1244:GLN:HG3	2.01	0.42
1:A:76:GLU:HB2	1:A:80:GLU:HB2	2.01	0.42
3:J:907:HIS:CG	3:J:908:ILE:N	2.88	0.42
5:L:316:PHE:CE2	5:L:334:SER:HA	2.55	0.42
1:B:101:THR:OG1	1:B:116:THR:OG1	2.30	0.42
3:D:1360:GLY:HA2	4:E:17:PHE:CE1	2.56	0.41
5:F:316:PHE:CE2	5:F:334:SER:HA	2.55	0.41
3:D:195:GLU:HA	3:D:198:CYS:SG	2.60	0.41
2:C:1307:ASN:O	2:C:1311:GLY:N	2.53	0.41
2:I:675:ASP:HA	3:J:763:PHE:HZ	1.84	0.41
2:I:130:MET:SD	2:I:134:GLY:HA2	2.60	0.41
3:D:242:LEU:HA	3:D:243:PRO:HD3	1.92	0.41
1:B:83:LEU:CD1	3:D:528:THR:HA	2.48	0.41
2:C:1085:MET:HG2	2:C:1094:VAL:O	2.20	0.41
5:L:300:LYS:HB3	5:L:300:LYS:HE3	1.81	0.41
1:A:207:THR:HG23	1:A:209:GLY:H	1.86	0.41
1:B:37:HIS:CD2	2:C:1216:ARG:HG2	2.55	0.41
5:L:311:THR:HG21	5:L:348:GLU:CD	2.40	0.41
2:I:1187:PHE:HZ	3:J:772:TYR:CG	2.37	0.41
1:G:179:PRO:HA	1:G:208:ASN:ND2	2.36	0.41
3:D:46:TYR:HB3	5:F:451:ARG:O	2.20	0.41
2:I:1244:HIS:HB2	2:I:1265:PHE:CD1	2.55	0.41
3:D:573:THR:O	3:D:577:ALA:N	2.42	0.41
4:K:40:PRO:C	4:K:42:GLU:H	2.23	0.41
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.19	0.41
2:C:176:ILE:HD12	2:C:184:LEU:HD23	2.02	0.41
2:I:151:ARG:H	2:I:151:ARG:HG2	1.34	0.41
3:J:419:HIS:O	3:J:439:PRO:HD2	2.21	0.41
2:I:1186:VAL:HG13	2:I:1187:PHE:CD1	2.50	0.41
3:J:452:LEU:HG	3:J:625:MET:CE	2.48	0.41
5:F:354:THR:CG2	5:F:357:GLN:HE21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:548:LEU:HA	5:F:551:LEU:HD21	2.03	0.41
5:L:276:MET:SD	5:L:279:ARG:NH2	2.93	0.41
2:I:145:ILE:HB	2:I:456:VAL:HG13	2.02	0.41
3:D:1169:THR:HA	3:D:1174:ARG:CB	2.50	0.41
5:F:530:LEU:HA	5:F:531:PRO:HD3	1.88	0.41
3:D:597:GLY:O	3:D:601:ILE:N	2.46	0.41
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.19	0.41
2:I:474:ALA:HB1	2:I:478:ARG:NH2	2.34	0.41
3:J:746:LEU:N	3:J:746:LEU:HD22	2.35	0.41
5:F:559:LEU:O	5:F:563:PHE:HD2	2.04	0.41
1:A:29:GLU:HG3	1:A:30:PRO:HD2	2.03	0.41
2:I:27:LEU:HD11	2:I:663:VAL:HG21	2.03	0.41
1:H:129:VAL:HG11	1:H:132:HIS:CE1	2.56	0.41
3:D:187:ALA:O	3:D:191:SER:HB2	2.21	0.41
1:G:75:GLN:HB3	1:G:132:HIS:HB2	2.02	0.41
2:I:1289:GLU:HB3	2:I:1294:LYS:HD2	2.01	0.41
6:N:4:D4P:HA	6:N:5:MEA:HC1	1.57	0.41
2:I:690:VAL:HA	2:I:691:PRO:HD3	1.96	0.41
3:J:775:SER:O	3:J:778:GLY:N	2.54	0.41
1:H:88:LEU:HD23	1:H:88:LEU:HA	1.91	0.41
2:I:448:LEU:HD23	2:I:448:LEU:HA	1.88	0.41
3:J:738:ARG:NH2	6:N:1:28H:OCD	2.53	0.41
3:J:816:THR:CG2	3:J:889:ASP:HB3	2.51	0.41
5:F:344:LEU:HA	5:F:344:LEU:HD12	1.90	0.41
5:F:440:THR:O	5:F:443:ILE:HG12	2.21	0.41
5:L:337:VAL:O	5:L:341:LEU:HG	2.21	0.41
5:L:379:MET:HG2	5:L:416:VAL:HG13	2.03	0.41
3:D:261:ALA:HA	5:F:505:ILE:O	2.21	0.41
1:H:56:VAL:HG12	1:H:173:VAL:HG11	2.02	0.41
1:G:179:PRO:HA	1:G:208:ASN:HD21	1.86	0.41
1:B:287:VAL:O	1:B:291:LYS:HG3	2.21	0.41
3:J:418:GLU:O	3:J:481:ARG:NH1	2.54	0.41
5:F:355:ILE:HD12	5:F:356:GLU:H	1.85	0.41
2:I:682:GLY:O	2:I:686:GLN:HG3	2.21	0.41
5:F:269:LEU:O	5:F:272:SER:HB3	2.21	0.41
3:J:813:ASP:HB2	3:J:897:HIS:HD2	1.86	0.41
1:G:219:ARG:O	1:G:223:ILE:HG13	2.20	0.41
5:F:352:GLY:O	5:F:353:LEU:HD23	2.21	0.41
5:F:143:TYR:OH	5:F:265:GLN:OE1	2.18	0.41
3:J:233:LYS:HB2	3:J:236:TRP:CE2	2.56	0.41
5:F:585:GLU:OE1	5:F:588:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:527:LEU:CB	3:D:533:ALA:HB2	2.51	0.41
3:D:739:GLN:CA	3:D:739:GLN:OE1	2.64	0.41
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.56	0.41
5:F:355:ILE:HD12	5:F:356:GLU:HG3	2.03	0.41
5:L:134:VAL:HG11	5:L:266:PHE:CE1	2.56	0.41
2:I:61:SER:OG	2:I:62:TYR:N	2.53	0.41
2:C:1222:GLU:OE2	3:D:512:TYR:OH	2.19	0.41
2:I:972:PHE:HB3	2:I:994:ARG:HH21	1.86	0.41
5:L:120:ALA:HA	5:L:123:ILE:HD12	2.03	0.41
2:C:24:VAL:HA	2:C:25:PRO:HD3	1.93	0.41
5:L:245:ALA:O	5:L:249:ILE:HG13	2.20	0.41
2:C:796:LEU:N	2:C:1231:TYR:HH	2.18	0.40
2:C:38:PHE:HA	2:C:48:GLY:HA2	2.04	0.40
1:H:68:TYR:O	1:H:68:TYR:CG	2.73	0.40
5:L:420:GLU:HB2	5:L:423:ARG:HH11	1.86	0.40
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.51	0.40
2:C:957:LYS:HA	2:C:1029:LEU:HD11	2.03	0.40
2:I:677:ASN:H	2:I:677:ASN:ND2	2.18	0.40
2:I:960:LEU:HD22	2:I:1029:LEU:HD12	2.03	0.40
3:J:261:ALA:HA	5:L:505:ILE:O	2.21	0.40
2:I:205:PRO:O	2:I:208:ILE:HG22	2.21	0.40
2:I:213:LEU:HD13	2:I:422:LYS:HB2	2.03	0.40
2:C:373:GLY:HA3	5:F:99:ARG:NH1	2.37	0.40
3:J:141:PHE:HB3	3:J:293:ARG:HD3	2.02	0.40
3:J:704:GLU:O	3:J:715:LYS:HA	2.21	0.40
2:I:836:LEU:HB3	2:I:918:LEU:HD21	2.02	0.40
2:C:52:ALA:O	2:C:56:VAL:HG23	2.20	0.40
5:F:551:LEU:HD23	5:F:556:ALA:HB2	2.03	0.40
2:C:821:ARG:HA	2:C:824:GLN:HB2	2.04	0.40
2:C:392:GLU:HA	2:C:395:TYR:O	2.21	0.40
3:J:1196:LEU:CB	3:J:1211:SER:HA	2.51	0.40
5:F:337:VAL:O	5:F:341:LEU:HG	2.22	0.40
2:I:802:VAL:HG12	2:I:1228:GLY:O	2.22	0.40
2:I:797:GLY:N	2:I:1231:TYR:OH	2.54	0.40
5:F:598:LEU:HD23	5:F:598:LEU:HA	1.90	0.40
5:L:271:ASN:O	5:L:275:VAL:HG23	2.22	0.40
2:C:1247:SER:HB3	3:D:375:GLU:O	2.21	0.40
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.89	0.40
3:J:706:VAL:O	3:J:714:GLU:N	2.30	0.40
1:B:32:GLU:HA	1:B:198:LEU:HD22	2.03	0.40
5:L:101:TYR:CE2	5:L:405:ILE:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:738:ARG:O	3:J:742:GLY:N	2.54	0.40
3:D:801:VAL:O	3:D:805:GLN:HB2	2.22	0.40
3:J:278:ARG:HD3	5:L:406:GLN:HB3	2.03	0.40
5:F:253:SER:O	5:F:257:LYS:HG3	2.21	0.40
5:F:311:THR:HG21	5:F:348:GLU:CD	2.41	0.40
2:C:948:ILE:O	2:C:952:GLN:HG3	2.21	0.40
5:L:415:ALA:HB2	5:L:434:TRP:HB2	2.04	0.40
2:C:225:PHE:CB	2:C:336:LEU:HD22	2.51	0.40
3:J:1224:ARG:HB3	3:J:1228:ALA:CB	2.51	0.40
5:F:138:PRO:O	5:F:142:THR:HG23	2.21	0.40
3:J:264:ASP:HB3	3:J:324:LEU:HB3	2.03	0.40
3:J:265:LEU:HA	3:J:265:LEU:HD23	1.87	0.40
1:G:170:ARG:NE	1:G:170:ARG:HA	2.37	0.40
3:D:910:ASN:HB3	4:E:15:ASN:HA	2.03	0.40
3:J:1291:GLU:O	3:J:1295:ASN:HB2	2.22	0.40
3:D:740:LEU:O	3:D:764:ARG:HB2	2.21	0.40
2:C:1150:ASP:HA	2:C:1153:ALA:CB	2.51	0.40
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.61	0.40
1:G:151:GLY:O	1:G:177:TYR:HB2	2.21	0.40
3:D:50:LYS:HD3	3:D:50:LYS:HA	1.84	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:218:ARG:NH2	5:L:149:ASP:OD1[1_545]	2.05	0.15
1:B:292:THR:O	1:H:68:TYR:OH[4_555]	2.19	0.01

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	292/335 (87%)	261 (89%)	19 (6%)	12 (4%)	3 36
1	B	281/335 (84%)	252 (90%)	13 (5%)	16 (6%)	2 28
1	G	212/335 (63%)	193 (91%)	14 (7%)	5 (2%)	7 49
1	H	211/335 (63%)	193 (92%)	13 (6%)	5 (2%)	7 49
2	C	1338/1342 (100%)	1265 (94%)	55 (4%)	18 (1%)	15 59
2	I	1338/1342 (100%)	1265 (94%)	54 (4%)	19 (1%)	14 58
3	D	1144/1407 (81%)	1027 (90%)	77 (7%)	40 (4%)	4 41
3	J	1137/1407 (81%)	1029 (90%)	60 (5%)	48 (4%)	3 35
4	E	87/91 (96%)	70 (80%)	8 (9%)	9 (10%)	1 12
4	K	73/91 (80%)	58 (80%)	10 (14%)	5 (7%)	1 24
5	F	456/613 (74%)	431 (94%)	19 (4%)	6 (1%)	15 59
5	L	456/613 (74%)	430 (94%)	18 (4%)	8 (2%)	11 54
All	All	7025/8246 (85%)	6474 (92%)	360 (5%)	191 (3%)	6 46

All (191) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	93	GLN
1	A	188	GLU
1	A	229	GLU
1	A	320	ASN
1	A	322	PRO
1	A	323	PRO
1	B	8	PHE
1	B	11	PRO
1	B	13	LEU
1	B	30	PRO
1	B	93	GLN
1	B	188	GLU
1	B	195	ARG
1	B	320	ASN
1	B	322	PRO
2	C	63	SER
2	C	110	PRO
2	C	214	ASN
2	C	346	TYR
2	C	748	ILE
3	D	151	MET

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Mol	Chain	Res	Type
3	D	407	VAL
3	D	539	SER
3	D	559	ALA
3	D	588	PRO
3	D	744	ARG
3	D	825	VAL
3	D	833	GLU
3	D	834	PRO
3	D	851	PRO
3	D	880	VAL
3	D	1149	ARG
3	D	1153	PRO
3	D	1168	GLU
3	D	1169	THR
3	D	1177	ILE
3	D	1185	PRO
3	D	1191	PRO
4	E	4	VAL
4	E	16	ARG
4	E	34	GLY
4	E	36	ASP
4	E	37	PRO
4	E	40	PRO
5	F	488	LEU
5	F	490	PRO
1	G	30	PRO
1	G	93	GLN
1	G	188	GLU
1	G	231	PHE
1	H	30	PRO
1	H	93	GLN
1	H	188	GLU
2	I	106	GLU
2	I	110	PRO
2	I	214	ASN
2	I	346	TYR
2	I	748	ILE
3	J	407	VAL
3	J	528	THR
3	J	539	SER
3	J	564	VAL
3	J	587	LEU

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Mol	Chain	Res	Type
3	J	588	PRO
3	J	744	ARG
3	J	833	GLU
3	J	835	LEU
3	J	851	PRO
3	J	859	PRO
3	J	880	VAL
3	J	1149	ARG
3	J	1153	PRO
3	J	1168	GLU
3	J	1176	VAL
3	J	1185	PRO
3	J	1191	PRO
3	J	1202	GLU
3	J	1209	VAL
3	J	1214	PRO
3	J	1215	GLU
4	K	34	GLY
4	K	36	ASP
4	K	37	PRO
4	K	39	VAL
5	L	488	LEU
5	L	490	PRO
1	A	319	GLU
1	B	7	GLU
1	B	191	ARG
1	B	192	VAL
1	B	319	GLU
2	C	109	ALA
2	C	746	ALA
2	C	909	LYS
2	C	1040	ASP
3	D	420	PRO
3	D	564	VAL
3	D	587	LEU
3	D	776	THR
3	D	906	GLY
3	D	1155	ILE
3	D	1190	ILE
5	F	307	THR
5	F	606	VAL
2	I	746	ALA

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Mol	Chain	Res	Type
2	I	891	GLY
2	I	910	ALA
2	I	941	LYS
3	J	151	MET
3	J	179	LYS
3	J	420	PRO
3	J	556	GLU
3	J	560	ASN
3	J	593	ASN
3	J	776	THR
3	J	906	GLY
3	J	1213	GLY
5	L	307	THR
5	L	384	LEU
5	L	606	VAL
1	A	33	ARG
1	A	192	VAL
1	B	193	GLU
1	B	229	GLU
2	C	925	SER
2	C	1204	LEU
3	D	718	SER
3	D	859	PRO
3	D	1150	PRO
4	E	60	ASN
5	F	384	LEU
2	I	925	SER
3	J	557	LYS
3	J	596	LEU
3	J	718	SER
3	J	1160	SER
3	J	1203	ARG
5	L	212	ILE
5	L	611	LEU
1	A	248	GLU
2	C	49	LEU
2	C	1155	VAL
2	C	1164	PHE
3	D	818	GLU
3	D	1176	VAL
4	E	79	GLU
4	E	80	LEU

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Mol	Chain	Res	Type
2	I	43	PRO
2	I	162	GLY
2	I	908	GLU
2	I	1203	ASP
2	I	1204	LEU
3	J	145	VAL
3	J	818	GLU
3	J	1150	PRO
3	J	1190	ILE
4	K	45	LYS
2	C	152	SER
2	C	1041	ASP
2	C	1181	PRO
2	C	1203	ASP
3	D	555	TYR
3	D	828	GLY
3	D	858	VAL
3	D	1208	ASP
3	D	1212	ASP
1	G	49	SER
1	H	49	SER
2	I	152	SER
2	I	1164	PHE
2	I	1181	PRO
1	A	49	SER
1	B	49	SER
3	D	1213	GLY
5	F	214	PRO
2	I	1179	GLY
3	J	322	ARG
3	D	856	ILE
3	J	823	THR
3	J	834	PRO
3	J	856	ILE
1	H	52	PRO
3	J	647	PRO
3	J	1159	ILE
3	J	1177	ILE
3	D	582	ILE
3	D	909	ILE
5	L	500	ILE
3	D	647	PRO

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Mol	Chain	Res	Type
3	J	582	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	239/292 (82%)	220 (92%)	19 (8%)	15 54
1	B	233/292 (80%)	218 (94%)	15 (6%)	22 61
1	G	173/292 (59%)	161 (93%)	12 (7%)	19 59
1	H	171/292 (59%)	158 (92%)	13 (8%)	16 55
2	C	822/1157 (71%)	765 (93%)	57 (7%)	19 59
2	I	828/1157 (72%)	765 (92%)	63 (8%)	16 55
3	D	520/1168 (44%)	455 (88%)	65 (12%)	6 32
3	J	518/1168 (44%)	452 (87%)	66 (13%)	5 31
4	E	10/75 (13%)	10 (100%)	0	100 100
4	K	9/75 (12%)	8 (89%)	1 (11%)	8 38
5	F	348/540 (64%)	306 (88%)	42 (12%)	6 33
5	L	348/540 (64%)	305 (88%)	43 (12%)	6 32
6	M	2/2 (100%)	1 (50%)	1 (50%)	0 0
6	N	2/2 (100%)	1 (50%)	1 (50%)	0 0
All	All	4223/7052 (60%)	3825 (91%)	398 (9%)	11 45

All (398) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	29	GLU
1	A	30	PRO
1	A	31	LEU
1	A	67	GLU
1	A	88	LEU

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Mol	Chain	Res	Type
1	A	95	LYS
1	A	102	LEU
1	A	117	HIS
1	A	131	CYS
1	A	140	ILE
1	A	143	ARG
1	A	171	LEU
1	A	173	VAL
1	A	178	SER
1	A	210	THR
1	A	318	LEU
1	A	319	GLU
1	A	321	TRP
1	B	14	VAL
1	B	29	GLU
1	B	31	LEU
1	B	88	LEU
1	B	95	LYS
1	B	102	LEU
1	B	117	HIS
1	B	131	CYS
1	B	140	ILE
1	B	171	LEU
1	B	173	VAL
1	B	178	SER
1	B	318	LEU
1	B	319	GLU
1	B	321	TRP
2	C	15	PHE
2	C	24	VAL
2	C	55	SER
2	C	66	SER
2	C	150	HIS
2	C	151	ARG
2	C	374	GLU
2	C	378	ARG
2	C	451	ARG
2	C	456	VAL
2	C	473	ARG
2	C	478	ARG
2	C	525	THR
2	C	529	ARG

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Mol	Chain	Res	Type
2	C	538	LEU
2	C	542	ARG
2	C	547	VAL
2	C	552	PRO
2	C	554	HIS
2	C	574	SER
2	C	581	THR
2	C	595	THR
2	C	600	THR
2	C	602	GLU
2	C	610	GLU
2	C	629	PHE
2	C	635	THR
2	C	643	SER
2	C	666	SER
2	C	677	ASN
2	C	678	ARG
2	C	692	THR
2	C	694	ARG
2	C	731	ARG
2	C	761	GLN
2	C	776	PRO
2	C	818	VAL
2	C	845	LEU
2	C	893	THR
2	C	896	THR
2	C	902	LEU
2	C	903	ARG
2	C	911	SER
2	C	917	SER
2	C	936	ARG
2	C	1042	LEU
2	C	1056	VAL
2	C	1075	VAL
2	C	1191	LYS
2	C	1197	GLU
2	C	1226	THR
2	C	1239	VAL
2	C	1243	MET
2	C	1250	SER
2	C	1259	LEU
2	C	1298	VAL

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Mol	Chain	Res	Type
2	C	1341	ASP
3	D	26	SER
3	D	34	SER
3	D	42	GLU
3	D	58	CYS
3	D	70	CYS
3	D	92	VAL
3	D	93	THR
3	D	118	LYS
3	D	167	ASP
3	D	191	SER
3	D	193	ASP
3	D	232	ASN
3	D	250	ARG
3	D	254	PRO
3	D	262	THR
3	D	301	GLU
3	D	311	ARG
3	D	319	SER
3	D	352	ARG
3	D	392	THR
3	D	419	HIS
3	D	420	PRO
3	D	430	HIS
3	D	491	LEU
3	D	505	ASP
3	D	514	THR
3	D	612	LEU
3	D	616	PRO
3	D	635	SER
3	D	646	ILE
3	D	661	VAL
3	D	673	VAL
3	D	674	THR
3	D	690	ASN
3	D	721	SER
3	D	733	SER
3	D	739	GLN
3	D	740	LEU
3	D	746	LEU
3	D	753	SER
3	D	763	PHE

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Mol	Chain	Res	Type
3	D	764	ARG
3	D	767	LEU
3	D	769	VAL
3	D	781	LYS
3	D	783	LEU
3	D	785	ASP
3	D	786	THR
3	D	790	THR
3	D	810	THR
3	D	816	THR
3	D	842	ARG
3	D	862	THR
3	D	869	CYS
3	D	877	VAL
3	D	880	VAL
3	D	882	VAL
3	D	885	VAL
3	D	894	VAL
3	D	913	GLU
3	D	1226	VAL
3	D	1282	TYR
3	D	1316	THR
3	D	1353	VAL
3	D	1355	ARG
5	F	137	TYR
5	F	158	LEU
5	F	159	SER
5	F	218	ARG
5	F	228	TYR
5	F	250	LEU
5	F	262	VAL
5	F	264	LYS
5	F	266	PHE
5	F	273	MET
5	F	309	ASN
5	F	311	THR
5	F	333	VAL
5	F	336	GLU
5	F	354	THR
5	F	355	ILE
5	F	360	ASP
5	F	374	ARG

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Mol	Chain	Res	Type
5	F	383	ASN
5	F	395	THR
5	F	397	ARG
5	F	401	PHE
5	F	420	GLU
5	F	421	TYR
5	F	425	TYR
5	F	426	LYS
5	F	428	SER
5	F	437	GLN
5	F	443	ILE
5	F	479	THR
5	F	480	PRO
5	F	513	ASP
5	F	537	THR
5	F	544	THR
5	F	551	LEU
5	F	552	THR
5	F	554	ARG
5	F	569	THR
5	F	583	THR
5	F	584	ARG
5	F	586	ARG
5	F	597	LYS
1	G	14	VAL
1	G	29	GLU
1	G	30	PRO
1	G	88	LEU
1	G	95	LYS
1	G	102	LEU
1	G	117	HIS
1	G	131	CYS
1	G	140	ILE
1	G	171	LEU
1	G	173	VAL
1	G	210	THR
1	H	14	VAL
1	H	29	GLU
1	H	30	PRO
1	H	88	LEU
1	H	95	LYS
1	H	102	LEU

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Mol	Chain	Res	Type
1	H	117	HIS
1	H	131	CYS
1	H	140	ILE
1	H	171	LEU
1	H	173	VAL
1	H	208	ASN
1	H	211	ILE
2	I	15	PHE
2	I	24	VAL
2	I	27	LEU
2	I	55	SER
2	I	135	THR
2	I	150	HIS
2	I	151	ARG
2	I	374	GLU
2	I	378	ARG
2	I	451	ARG
2	I	456	VAL
2	I	473	ARG
2	I	478	ARG
2	I	525	THR
2	I	529	ARG
2	I	530	ILE
2	I	538	LEU
2	I	542	ARG
2	I	547	VAL
2	I	552	PRO
2	I	554	HIS
2	I	574	SER
2	I	581	THR
2	I	595	THR
2	I	600	THR
2	I	602	GLU
2	I	610	GLU
2	I	634	VAL
2	I	635	THR
2	I	637	ARG
2	I	657	THR
2	I	666	SER
2	I	678	ARG
2	I	694	ARG
2	I	731	ARG

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Mol	Chain	Res	Type
2	I	736	VAL
2	I	761	GLN
2	I	770	CYS
2	I	776	PRO
2	I	818	VAL
2	I	845	LEU
2	I	893	THR
2	I	896	THR
2	I	902	LEU
2	I	903	ARG
2	I	906	PHE
2	I	917	SER
2	I	936	ARG
2	I	942	ASP
2	I	1042	LEU
2	I	1056	VAL
2	I	1075	VAL
2	I	1184	THR
2	I	1191	LYS
2	I	1197	GLU
2	I	1226	THR
2	I	1239	VAL
2	I	1243	MET
2	I	1250	SER
2	I	1259	LEU
2	I	1262	LYS
2	I	1298	VAL
2	I	1341	ASP
3	J	26	SER
3	J	34	SER
3	J	42	GLU
3	J	58	CYS
3	J	92	VAL
3	J	93	THR
3	J	118	LYS
3	J	167	ASP
3	J	191	SER
3	J	193	ASP
3	J	210	SER
3	J	232	ASN
3	J	250	ARG
3	J	254	PRO

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Mol	Chain	Res	Type
3	J	262	THR
3	J	301	GLU
3	J	311	ARG
3	J	319	SER
3	J	352	ARG
3	J	392	THR
3	J	400	MET
3	J	401	VAL
3	J	402	GLU
3	J	419	HIS
3	J	430	HIS
3	J	505	ASP
3	J	514	THR
3	J	598	LYS
3	J	612	LEU
3	J	616	PRO
3	J	635	SER
3	J	646	ILE
3	J	661	VAL
3	J	673	VAL
3	J	674	THR
3	J	690	ASN
3	J	721	SER
3	J	733	SER
3	J	739	GLN
3	J	740	LEU
3	J	753	SER
3	J	763	PHE
3	J	764	ARG
3	J	767	LEU
3	J	769	VAL
3	J	781	LYS
3	J	783	LEU
3	J	785	ASP
3	J	786	THR
3	J	790	THR
3	J	816	THR
3	J	842	ARG
3	J	862	THR
3	J	864	LEU
3	J	868	TRP
3	J	869	CYS

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Mol	Chain	Res	Type
3	J	877	VAL
3	J	880	VAL
3	J	885	VAL
3	J	894	VAL
3	J	913	GLU
3	J	1226	VAL
3	J	1282	TYR
3	J	1316	THR
3	J	1353	VAL
3	J	1355	ARG
4	K	6	VAL
5	L	137	TYR
5	L	158	LEU
5	L	159	SER
5	L	210	ASN
5	L	211	SER
5	L	218	ARG
5	L	228	TYR
5	L	230	VAL
5	L	234	THR
5	L	250	LEU
5	L	262	VAL
5	L	264	LYS
5	L	266	PHE
5	L	273	MET
5	L	309	ASN
5	L	311	THR
5	L	333	VAL
5	L	336	GLU
5	L	354	THR
5	L	360	ASP
5	L	374	ARG
5	L	383	ASN
5	L	395	THR
5	L	397	ARG
5	L	401	PHE
5	L	420	GLU
5	L	421	TYR
5	L	422	ARG
5	L	425	TYR
5	L	426	LYS
5	L	428	SER

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Mol	Chain	Res	Type
5	L	437	GLN
5	L	479	THR
5	L	480	PRO
5	L	513	ASP
5	L	537	THR
5	L	552	THR
5	L	554	ARG
5	L	569	THR
5	L	584	ARG
5	L	586	ARG
5	L	589	GLN
5	L	597	LYS
6	M	2	THR
6	N	2	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	41	ASN
1	A	128	HIS
1	A	147	GLN
1	A	227	GLN
1	A	283	GLN
1	A	320	ASN
1	B	37	HIS
1	B	41	ASN
1	B	128	HIS
1	B	147	GLN
1	B	283	GLN
1	B	320	ASN
2	C	437	ASN
2	C	659	GLN
2	C	677	ASN
2	C	955	GLN
2	C	1013	GLN
2	C	1023	HIS
3	D	113	HIS
3	D	477	GLN
3	D	690	ASN
3	D	777	HIS
3	D	865	HIS

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Mol	Chain	Res	Type
3	D	897	HIS
3	D	1326	GLN
5	F	128	ASN
5	F	129	GLN
5	F	131	GLN
5	F	227	GLN
5	F	309	ASN
5	F	357	GLN
5	F	383	ASN
5	F	406	GLN
5	F	437	GLN
1	G	37	HIS
1	G	41	ASN
1	G	66	HIS
1	G	128	HIS
1	G	147	GLN
1	H	66	HIS
1	H	128	HIS
1	H	147	GLN
1	H	208	ASN
1	H	227	GLN
2	I	437	ASN
2	I	659	GLN
2	I	955	GLN
2	I	1013	GLN
2	I	1017	GLN
2	I	1023	HIS
2	I	1257	GLN
3	J	274	ASN
3	J	477	GLN
3	J	777	HIS
3	J	805	GLN
3	J	897	HIS
3	J	1326	GLN
5	L	128	ASN
5	L	129	GLN
5	L	131	GLN
5	L	227	GLN
5	L	357	GLN
5	L	383	ASN
5	L	437	GLN
5	L	446	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
6	28J	M	3	6	6,7,8	0.44	0	7,8,10	1.17	1 (14%)
6	D4P	M	4	6	10,11,12	4.40	2 (20%)	12,14,16	0.75	0
6	MEA	M	5	6	10,12,13	1.59	1 (10%)	10,14,16	1.13	1 (10%)
6	2TL	M	6	6	5,6,7	0.49	0	5,7,9	1.23	1 (20%)
6	28J	N	3	6	6,7,8	0.44	0	7,8,10	1.17	1 (14%)
6	D4P	N	4	6	10,11,12	4.39	2 (20%)	12,14,16	0.76	0
6	MEA	N	5	6	10,12,13	1.59	1 (10%)	10,14,16	1.13	1 (10%)
6	2TL	N	6	6	5,6,7	0.49	0	5,7,9	1.23	1 (20%)

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
6	28J	M	3	6	-	0/6/8/10	0/0/0/0
6	D4P	M	4	6	-	0/4/6/8	0/1/1/1
6	MEA	M	5	6	-	0/4/8/10	0/1/1/1
6	2TL	M	6	6	-	0/4/6/8	0/0/0/0
6	28J	N	3	6	-	0/6/8/10	0/0/0/0
6	D4P	N	4	6	-	0/4/6/8	0/1/1/1
6	MEA	N	5	6	-	0/4/8/10	0/1/1/1
6	2TL	N	6	6	-	0/4/6/8	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	4	D4P	C1-CA	-13.33	1.39	1.52
6	N	4	D4P	C1-CA	-13.32	1.39	1.52
6	N	5	MEA	CB-CG	-4.81	1.39	1.51
6	M	5	MEA	CB-CG	-4.80	1.39	1.51
6	M	4	D4P	CA-C	-3.78	1.39	1.50
6	N	4	D4P	CA-C	-3.76	1.39	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	5	MEA	CG-CB-CA	-2.74	109.53	114.26
6	N	5	MEA	CG-CB-CA	-2.73	109.55	114.26
6	N	6	2TL	CG2-CB-CA	-2.07	109.48	112.53
6	M	6	2TL	CG2-CB-CA	-2.06	109.50	112.53
6	M	3	28J	CB-CA-C	-2.05	109.50	112.79
6	N	3	28J	CB-CA-C	-2.04	109.51	112.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	3	28J	1	0
6	M	4	D4P	7	0
6	M	5	MEA	10	0
6	M	6	2TL	6	0
6	N	3	28J	1	0
6	N	4	D4P	7	0
6	N	5	MEA	9	0
6	N	6	2TL	6	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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

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	298/335 (88%)	0.30	21 (7%) 19 13	41, 129, 238, 393	0
1	B	287/335 (85%)	0.37	27 (9%) 11 7	58, 173, 336, 460	0
1	G	216/335 (64%)	0.58	26 (12%) 6 5	68, 183, 311, 358	0
1	H	215/335 (64%)	0.66	37 (17%) 2 2	79, 191, 326, 488	0
2	C	1340/1342 (99%)	0.11	71 (5%) 30 22	16, 113, 346, 550	1 (0%)
2	I	1340/1342 (99%)	0.48	146 (10%) 7 6	37, 162, 408, 550	1 (0%)
3	D	1150/1407 (81%)	-0.11	23 (2%) 68 57	19, 89, 227, 505	0
3	J	1143/1407 (81%)	-0.10	29 (2%) 61 48	31, 110, 251, 550	0
4	E	89/91 (97%)	-0.59	0 100 100	28, 105, 210, 326	0
4	K	75/91 (82%)	0.16	5 (6%) 21 13	91, 185, 373, 403	0
5	F	464/613 (75%)	0.18	28 (6%) 25 17	45, 151, 353, 550	0
5	L	464/613 (75%)	0.17	30 (6%) 22 14	53, 167, 378, 550	0
6	M	3/9 (33%)	-0.34	0 100 100	107, 107, 108, 111	0
6	N	3/9 (33%)	-0.66	0 100 100	130, 130, 134, 138	0
All	All	7087/8264 (85%)	0.16	443 (6%) 23 15	16, 134, 326, 550	2 (0%)

All (443) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1000	LEU	26.3
2	I	981	ALA	18.8
2	I	231	GLU	15.8
2	I	1001	GLY	11.8
2	I	332	ARG	11.5
2	C	287	VAL	11.1
2	I	982	GLY	10.8
2	I	980	VAL	10.7

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Mol	Chain	Res	Type	RSRZ
2	I	979	LEU	10.7
2	I	978	VAL	10.4
2	I	232	ILE	10.1
2	I	235	ASN	9.3
2	C	291	TYR	9.1
2	I	494	ASN	8.9
2	I	995	ASP	8.6
2	I	999	GLU	8.4
2	I	333	ILE	8.3
2	I	986	ALA	8.2
3	D	1204	VAL	7.8
2	C	292	ILE	7.8
2	I	976	ARG	7.7
2	C	322	LEU	7.3
2	I	1004	ASP	7.3
2	I	994	ARG	7.1
2	C	305	SER	7.1
2	I	969	ALA	7.0
2	I	489	PRO	6.9
5	F	355	ILE	6.8
2	I	974	ARG	6.8
2	C	288	PRO	6.7
2	I	1003	THR	6.6
2	I	230	PHE	6.6
2	I	970	GLY	6.5
5	L	340	ALA	6.5
2	I	334	GLU	6.4
2	C	252	SER	6.4
1	H	193	GLU	6.3
2	I	973	SER	6.2
2	I	234	ASP	6.2
2	C	251	ALA	6.1
1	H	192	VAL	6.1
2	I	122	VAL	6.0
5	L	355	ILE	6.0
2	I	977	ALA	6.0
2	I	1021	LEU	5.9
2	I	787	PRO	5.9
1	H	98	VAL	5.9
2	I	1005	GLU	5.7
5	F	319	ALA	5.5
2	C	286	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
2	I	975	ILE	5.5
2	I	987	GLU	5.5
2	I	482	GLY	5.4
2	C	253	PHE	5.4
3	J	1299	GLY	5.2
3	J	674	THR	5.2
2	I	998	LEU	5.1
2	I	121	GLU	5.1
2	I	68	LEU	5.1
2	I	495	ALA	5.0
2	I	311	CYS	5.0
1	G	205	MET	4.9
1	H	146	VAL	4.9
2	I	985	GLU	4.8
1	B	146	VAL	4.8
2	C	314	ASN	4.7
5	F	280	VAL	4.7
2	I	1020	GLU	4.7
2	I	1007	LYS	4.6
1	A	300	LEU	4.6
1	B	303	ILE	4.6
5	F	305	LEU	4.5
2	C	329	GLY	4.5
2	C	374	GLU	4.5
2	I	42	ASP	4.5
4	K	19	LEU	4.5
2	C	230	PHE	4.4
1	B	172	LEU	4.4
5	L	315	TRP	4.4
1	H	144	ILE	4.3
2	I	236	LYS	4.3
2	C	376	PRO	4.2
1	G	26	VAL	4.2
5	F	237	ALA	4.2
2	I	983	GLY	4.2
5	F	261	LEU	4.2
2	C	596	ASP	4.2
3	J	673	VAL	4.1
2	C	311	CYS	4.1
5	L	237	ALA	4.1
1	G	194	GLN	4.1
2	I	305	SER	4.0

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Mol	Chain	Res	Type	RSRZ
4	K	36	ASP	4.0
2	I	373	GLY	4.0
5	L	416	VAL	3.9
2	C	325	LEU	3.9
5	F	315	TRP	3.9
1	A	294	ASN	3.9
1	H	100	LEU	3.9
3	J	1203	ARG	3.9
5	F	354	THR	3.9
1	B	260	LEU	3.8
3	D	140	TYR	3.8
3	D	256	ASP	3.8
2	I	945	ALA	3.8
3	J	675	ALA	3.8
1	H	194	GLN	3.8
1	B	281	LEU	3.8
2	I	374	GLU	3.8
1	A	262	LEU	3.7
1	B	318	LEU	3.7
2	C	206	ALA	3.7
1	H	205	MET	3.7
2	C	331	LYS	3.7
1	H	90	VAL	3.7
2	I	322	LEU	3.7
2	I	299	LYS	3.6
2	I	1017	GLN	3.6
2	C	235	ASN	3.6
3	J	1214	PRO	3.6
2	C	1000	LEU	3.6
2	C	234	ASP	3.6
1	B	295	LEU	3.6
2	I	1018	TYR	3.6
2	I	474	ALA	3.6
2	I	1265	PHE	3.5
2	I	984	VAL	3.5
2	I	997	TRP	3.5
2	C	378	ARG	3.5
2	I	442	VAL	3.5
5	L	489	MET	3.5
2	I	246	LEU	3.5
2	I	972	PHE	3.5
1	G	17	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	I	198	ILE	3.5
5	L	412	LEU	3.5
5	F	318	ALA	3.5
5	L	287	ILE	3.4
2	I	493	ILE	3.4
1	G	35	PHE	3.4
5	L	165	PHE	3.4
2	C	184	LEU	3.4
2	C	236	LYS	3.4
3	J	1152	GLU	3.4
2	C	207	THR	3.4
2	C	370	MET	3.4
2	C	321	LEU	3.4
2	I	400	VAL	3.4
1	H	121	VAL	3.4
2	I	66	SER	3.4
5	L	420	GLU	3.3
3	J	650	LYS	3.3
3	J	1195	GLN	3.3
2	I	224	PHE	3.3
1	G	13	LEU	3.3
2	I	492	MET	3.3
2	I	107	ARG	3.3
1	B	117	HIS	3.3
2	I	1002	LEU	3.2
1	H	149	GLY	3.2
2	I	718	ALA	3.2
5	L	310	GLU	3.2
4	K	35	LYS	3.2
1	A	266	SER	3.2
2	C	1265	PHE	3.2
1	H	101	THR	3.2
2	I	944	ARG	3.2
5	F	344	LEU	3.2
2	I	203	LYS	3.2
5	L	234	THR	3.2
1	G	25	LYS	3.2
2	I	255	ILE	3.2
1	B	98	VAL	3.1
4	K	37	PRO	3.1
1	G	203	ILE	3.1
5	L	293	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	350	THR	3.1
2	I	971	LEU	3.1
5	L	336	GLU	3.1
4	K	18	ASP	3.1
2	C	165	HIS	3.1
2	I	233	ARG	3.1
3	J	1198	VAL	3.1
1	G	47	LEU	3.1
2	C	194	LEU	3.1
1	G	148	ARG	3.0
2	I	41	GLN	3.0
3	J	76	LYS	3.0
2	I	301	TYR	3.0
2	C	233	ARG	3.0
3	J	670	SER	3.0
3	D	878	ASP	3.0
2	I	263	VAL	3.0
1	H	26	VAL	3.0
2	C	208	ILE	3.0
2	I	292	ILE	3.0
3	J	77	ARG	3.0
1	A	318	LEU	3.0
3	D	1175	LEU	3.0
2	C	318	SER	3.0
2	C	285	ILE	2.9
3	J	232	ASN	2.9
2	C	250	THR	2.9
1	A	270	LEU	2.9
2	I	340	ASP	2.9
1	A	121	VAL	2.9
1	H	181	GLU	2.9
2	I	1160	ASP	2.9
2	I	989	LEU	2.9
3	J	206	ASN	2.9
5	L	309	ASN	2.9
2	C	332	ARG	2.9
3	D	206	ASN	2.9
5	L	306	PHE	2.9
1	H	92	VAL	2.9
2	C	373	GLY	2.9
1	A	295	LEU	2.9
2	C	347	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	205	PRO	2.9
1	A	131	CYS	2.9
2	I	1014	LEU	2.9
1	A	275	ILE	2.9
2	C	198	ILE	2.9
2	I	478	ARG	2.8
1	G	197	ASP	2.8
3	J	872	LEU	2.8
1	H	31	LEU	2.8
2	I	282	VAL	2.8
2	I	1266	GLY	2.8
1	A	205	MET	2.8
1	G	91	ARG	2.8
2	I	1296	ASP	2.8
5	L	286	LEU	2.8
1	A	110	VAL	2.8
1	G	202	VAL	2.8
1	H	171	LEU	2.8
2	C	56	VAL	2.8
2	I	1029	LEU	2.8
1	G	54	CYS	2.7
3	J	1212	ASP	2.7
3	D	90	VAL	2.7
2	I	1022	LYS	2.7
3	D	204	GLU	2.7
2	C	166	SER	2.7
2	I	1006	GLU	2.7
2	I	73	TYR	2.7
2	I	1263	ALA	2.7
5	F	316	PHE	2.7
1	B	283	GLN	2.7
2	I	240	GLU	2.7
2	I	641	GLU	2.7
3	J	1289	ASN	2.7
1	A	98	VAL	2.7
2	C	942	ASP	2.7
3	D	62	PHE	2.7
2	I	243	PRO	2.7
5	L	337	VAL	2.7
2	C	264	GLU	2.7
2	C	382	GLU	2.7
1	B	282	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	J	1161	GLY	2.7
2	I	104	ILE	2.6
2	I	269	ILE	2.6
5	L	423	ARG	2.6
3	D	1173	ARG	2.6
2	C	258	ASN	2.6
2	C	290	GLU	2.6
1	H	56	VAL	2.6
2	I	1010	GLN	2.6
5	L	284	GLU	2.6
2	I	103	VAL	2.6
2	C	482	GLY	2.6
2	I	449	GLY	2.6
2	I	204	LEU	2.6
1	G	68	TYR	2.6
1	H	123	ILE	2.6
2	I	252	SER	2.6
3	J	1300	ALA	2.6
5	F	317	ASN	2.6
3	D	932	MET	2.6
5	F	516	ASP	2.6
2	I	450	ASN	2.6
5	L	344	LEU	2.6
1	A	30	PRO	2.5
1	H	15	ASP	2.5
5	F	337	VAL	2.5
2	I	253	PHE	2.5
1	B	323	PRO	2.5
5	F	336	GLU	2.5
5	F	584	ARG	2.5
2	C	113	THR	2.5
2	I	988	LYS	2.5
1	A	260	LEU	2.5
2	I	1264	GLN	2.5
1	H	27	THR	2.5
5	F	515	GLU	2.5
1	B	201	LEU	2.5
1	G	21	SER	2.5
3	D	543	SER	2.5
3	J	24	LEU	2.5
2	C	209	ILE	2.5
2	I	1067	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	I	262	TYR	2.5
1	H	13	LEU	2.5
1	H	145	LYS	2.5
2	I	894	GLN	2.5
1	B	144	ILE	2.5
5	L	415	ALA	2.5
3	D	139	LEU	2.4
2	C	232	ILE	2.4
3	J	1213	GLY	2.4
3	J	1197	ASN	2.4
2	I	404	LYS	2.4
2	I	937	ASP	2.4
1	G	43	LEU	2.4
3	D	209	ASN	2.4
2	I	46	GLN	2.4
2	I	727	VAL	2.4
2	I	1016	GLU	2.4
3	D	1215	GLU	2.4
1	A	54	CYS	2.4
3	D	825	VAL	2.4
2	I	722	GLY	2.4
1	A	97	GLU	2.4
3	D	136	GLU	2.4
2	C	265	LYS	2.4
3	D	1174	ARG	2.4
1	B	289	LEU	2.4
2	I	237	LEU	2.4
1	B	50	SER	2.4
1	B	296	GLY	2.3
2	I	100	LEU	2.3
2	I	420	LEU	2.3
1	B	314	LEU	2.3
2	C	239	MET	2.3
1	H	95	LYS	2.3
1	H	191	ARG	2.3
2	I	265	LYS	2.3
3	J	1215	GLU	2.3
2	I	935	THR	2.3
2	I	539	THR	2.3
3	J	686	TRP	2.3
3	D	1205	GLU	2.3
5	F	310	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	306	THR	2.3
5	L	311	THR	2.3
1	H	51	MET	2.3
2	C	204	LEU	2.3
3	D	858	VAL	2.3
1	A	96	ASP	2.3
2	I	966	ILE	2.3
1	B	297	LYS	2.2
1	A	267	ALA	2.2
2	I	771	VAL	2.2
1	B	171	LEU	2.2
1	G	36	GLY	2.2
5	F	277	MET	2.2
5	F	157	ARG	2.2
1	B	78	ILE	2.2
2	C	186	PHE	2.2
5	F	463	LEU	2.2
3	J	512	TYR	2.2
1	B	284	ARG	2.2
1	H	208	ASN	2.2
2	I	911	SER	2.2
2	I	1295	SER	2.2
5	F	358	VAL	2.2
1	G	195	ARG	2.2
2	C	259	GLY	2.2
2	I	1025	PHE	2.2
2	I	98	VAL	2.2
1	H	61	ILE	2.2
2	I	196	VAL	2.2
2	I	220	ILE	2.2
2	C	375	PRO	2.2
3	J	732	GLY	2.2
2	I	599	VAL	2.2
2	I	277	LEU	2.2
1	B	97	GLU	2.2
5	F	420	GLU	2.2
5	L	288	MET	2.2
5	L	487	MET	2.2
5	F	293	GLU	2.2
1	G	186	ASN	2.2
1	B	299	SER	2.2
1	H	28	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	377	THR	2.1
1	G	24	ALA	2.1
2	I	298	ALA	2.1
1	H	12	ARG	2.1
2	I	229	ILE	2.1
2	I	686	GLN	2.1
5	L	347	ILE	2.1
2	I	331	LYS	2.1
3	J	663	GLU	2.1
5	F	325	PRO	2.1
1	G	144	ILE	2.1
1	G	204	GLU	2.1
2	I	1072	ASN	2.1
3	D	394	ILE	2.1
5	L	490	PRO	2.1
2	I	69	GLN	2.1
2	C	176	ILE	2.1
1	H	204	GLU	2.1
2	C	498	ILE	2.1
2	C	263	VAL	2.1
3	D	1169	THR	2.1
1	H	182	ARG	2.1
2	C	944	ARG	2.1
5	L	560	ARG	2.1
2	C	257	ALA	2.1
2	I	1190	ALA	2.1
2	I	67	GLU	2.1
5	L	427	PHE	2.1
5	F	101	TYR	2.1
5	F	234	THR	2.1
1	B	67	GLU	2.1
1	H	97	GLU	2.1
1	G	90	VAL	2.1
1	H	59	VAL	2.1
2	C	464	PHE	2.1
1	B	139	SER	2.1
1	H	16	ILE	2.1
1	A	227	GLN	2.1
2	I	471	VAL	2.1
1	B	212	ASP	2.1
2	I	753	LEU	2.1
1	G	211	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	990	ASP	2.1
3	D	675	ALA	2.1
5	L	408	GLY	2.1
2	C	354	ASP	2.1
2	I	317	LEU	2.0
2	C	1018	TYR	2.0
2	I	696	ASP	2.0
3	J	524	GLY	2.0
1	H	180	VAL	2.0
2	I	169	LYS	2.0
1	G	193	GLU	2.0
1	A	259	ASP	2.0
1	H	142	MET	2.0
2	C	487	LEU	2.0
5	F	590	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
6	28J	N	3	8/9	0.95	0.18	-	106,127,131,132	0
6	28J	M	3	8/9	0.97	0.28	-	97,105,111,114	0
6	MEA	M	5	12/13	0.91	0.27	-	79,91,106,106	0
6	D4P	N	4	11/12	0.92	0.16	-	133,140,153,159	0
6	MEA	N	5	12/13	0.82	0.32	-	109,123,128,130	0
6	2TL	M	6	7/8	0.96	0.20	-	91,110,113,123	0
6	2TL	N	6	7/8	0.90	0.18	-	124,127,132,147	0
6	D4P	M	4	11/12	0.93	0.18	-	102,118,135,137	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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
8	ZN	J	2002	1/1	0.97	0.25	-0.09	80,80,80,80	0
8	ZN	D	2002	1/1	0.98	0.23	-0.56	64,64,64,64	0
8	ZN	D	2001	1/1	0.93	0.10	-0.79	87,87,87,87	0
8	ZN	J	2001	1/1	0.97	0.08	-1.83	106,106,106,106	0
7	MG	J	2000	1/1	0.79	0.82	-	98,98,98,98	0
7	MG	D	2000	1/1	0.88	0.72	-	258,258,258,258	0

6.5 Other polymers

There are no such residues in this entry.