



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:33 PM UTC

PDB ID : 4MEY / pdb_00004mey
Title : Crystal structure of Escherichia coli RNA polymerase holoenzyme
Authors : Feng, Y.; Zhang, Y.; Arnold, E.; Ebright, R.H.
Deposited on : 2013-08-27
Resolution : 3.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

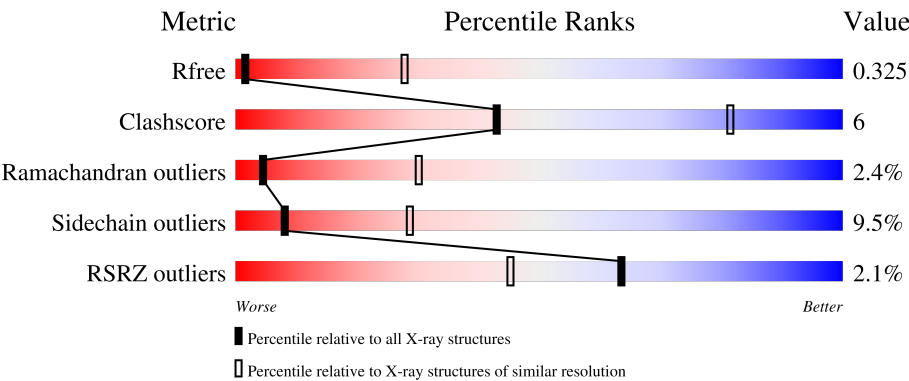
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1022 (4.12-3.76)
Clashscore	190562	1000 (4.10-3.78)
Ramachandran outliers	187476	1009 (4.12-3.76)
Sidechain outliers	187428	1002 (4.12-3.76)
RSRZ outliers	180081	1022 (4.12-3.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	335	0% 68%17%11%
1	B	335	4% 66%16%14%
1	G	335	0% 51%11%36%
1	H	335	2% 49%13%36%
2	C	1342	2% 81%18%

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Mol	Chain	Length	Quality of chain
2	I	1342	3% 81% 18%
3	D	1407	% 65% 15% 18%
3	J	1407	2% 65% 15% 19%
4	E	91	% 77% 16%
4	K	91	3% 67% 12% 18%
5	F	613	% 59% 15% 24%
5	L	613	% 59% 15% 24%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49826 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	1147	Total	C	N	O	S	0	0	0
			7549	4756	1355	1411	27			
3	J	1140	Total	C	N	O	S	0	0	0
			7512	4733	1348	1404	27			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		

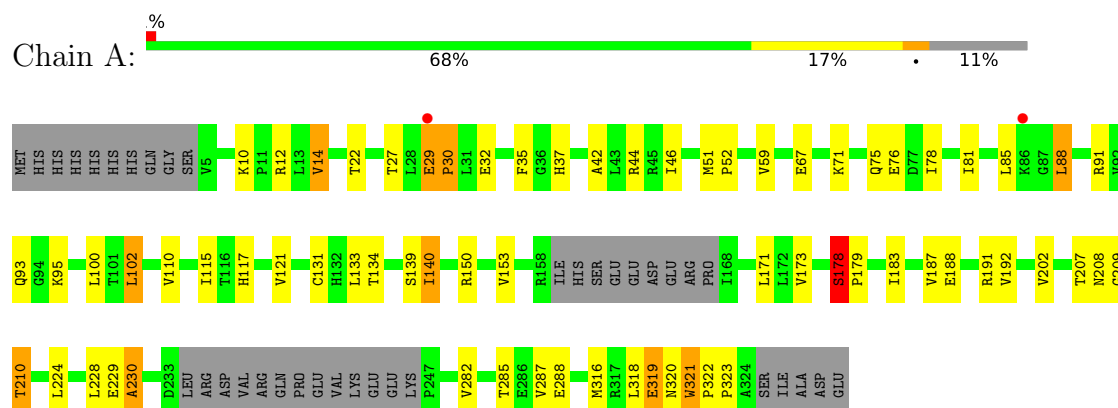
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

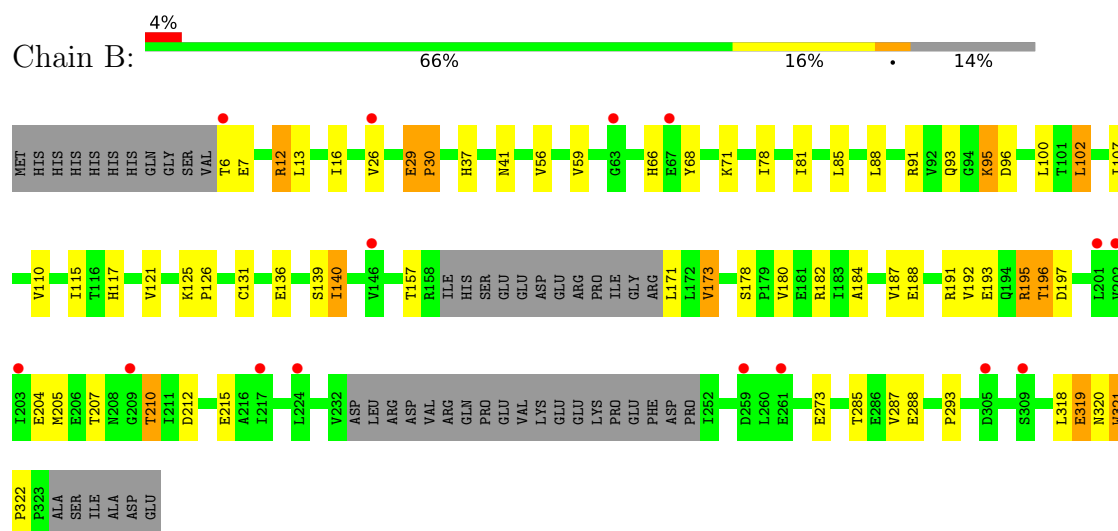
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

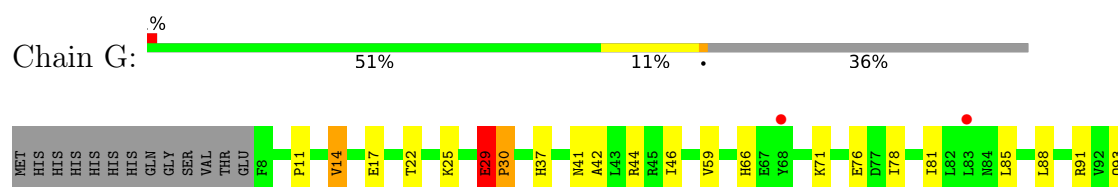
• Molecule 1: DNA-directed RNA polymerase subunit alpha

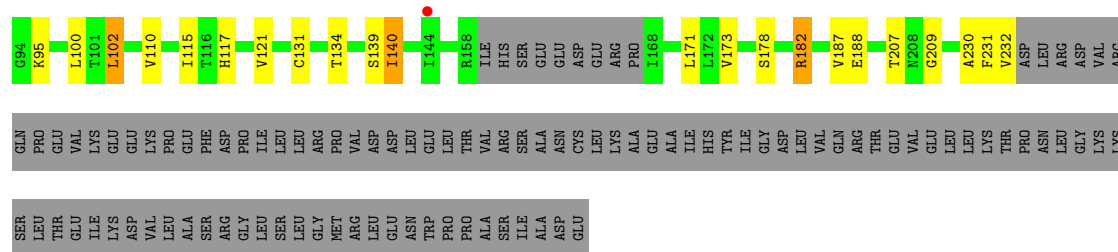


• Molecule 1: DNA-directed RNA polymerase subunit alpha

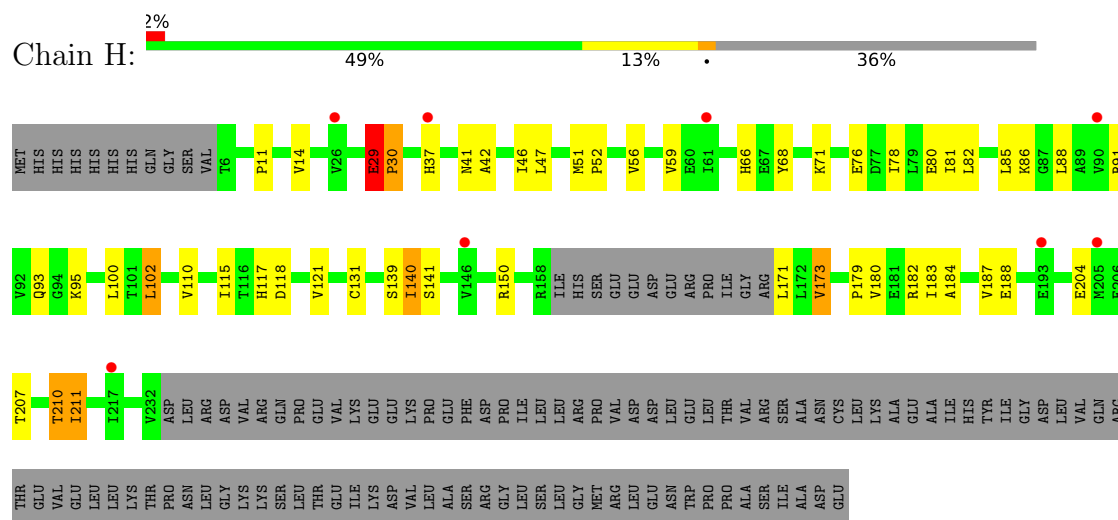


• Molecule 1: DNA-directed RNA polymerase subunit alpha

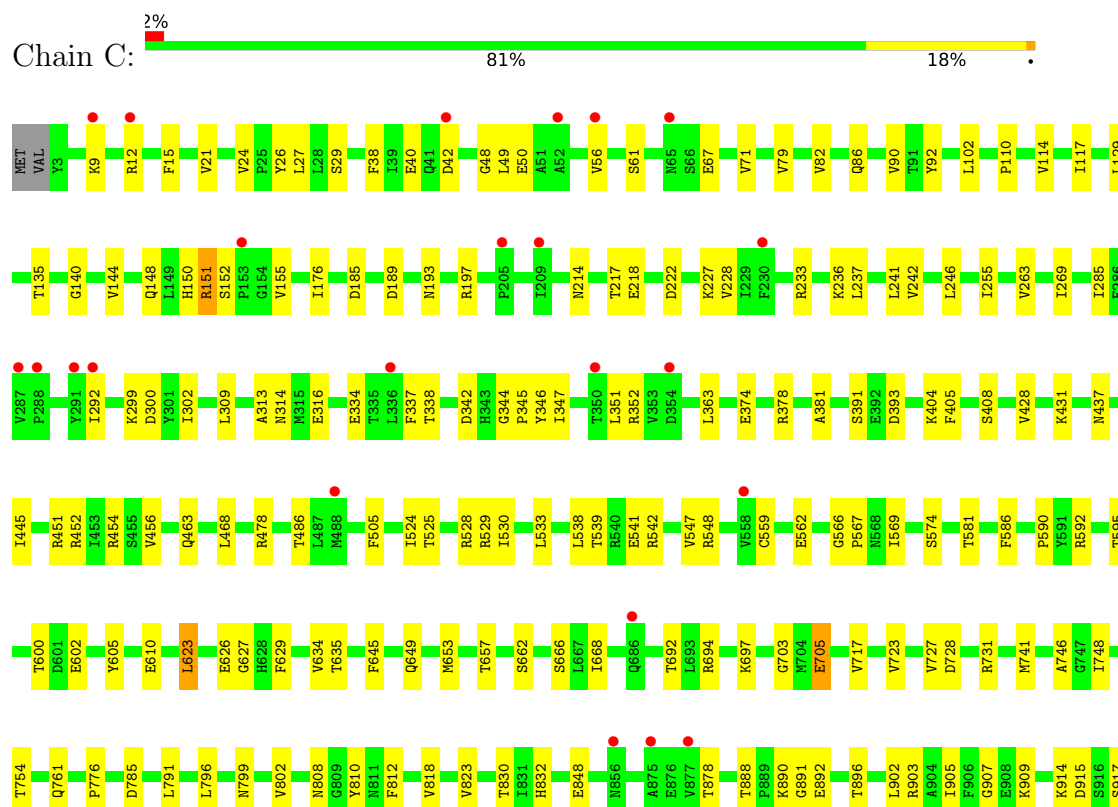


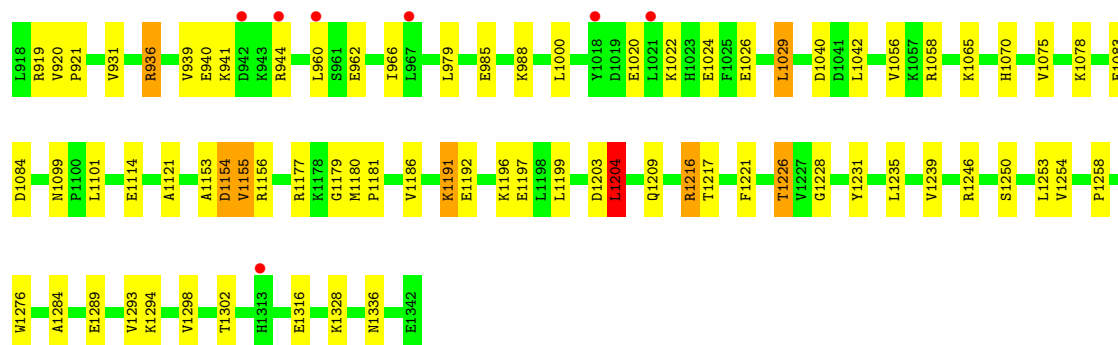


• Molecule 1: DNA-directed RNA polymerase subunit alpha

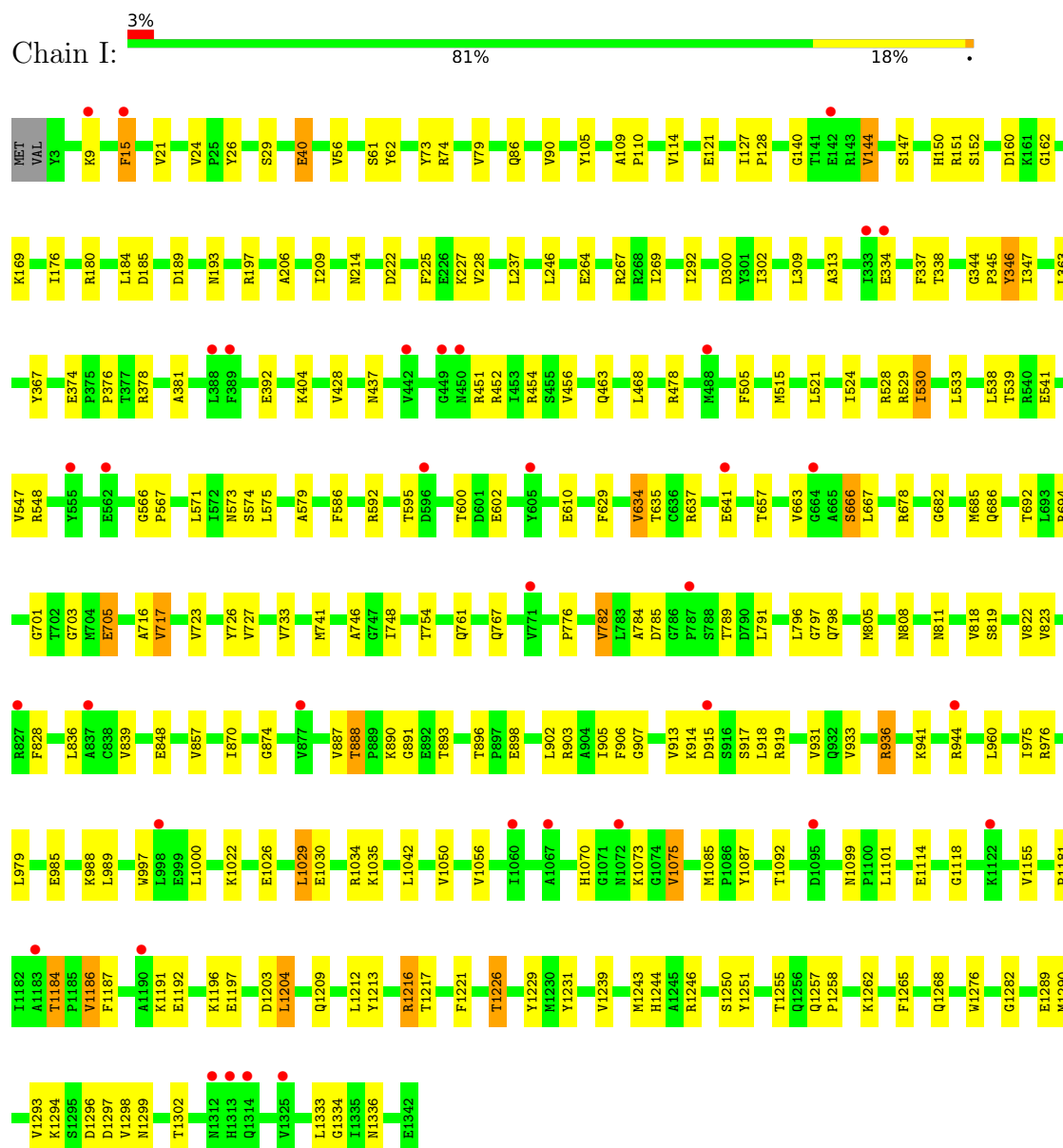


• Molecule 2: DNA-directed RNA polymerase subunit beta



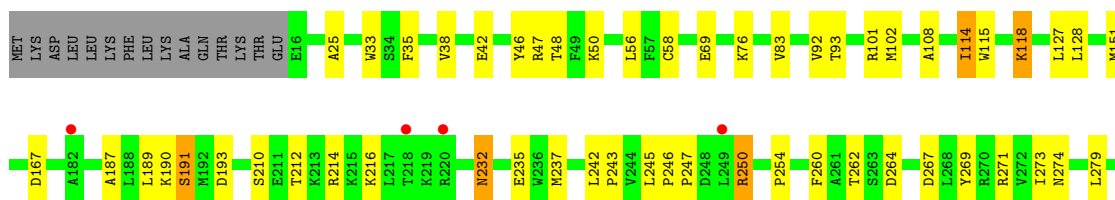


• Molecule 2: DNA-directed RNA polymerase subunit beta

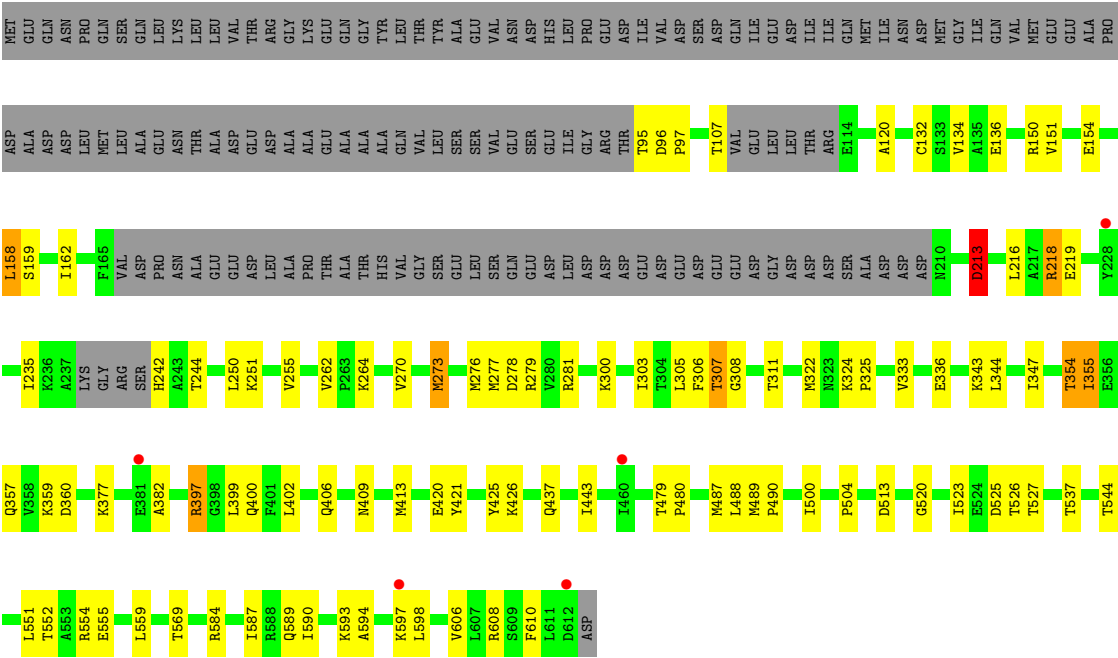


• Molecule 3: DNA-directed RNA polymerase subunit beta'

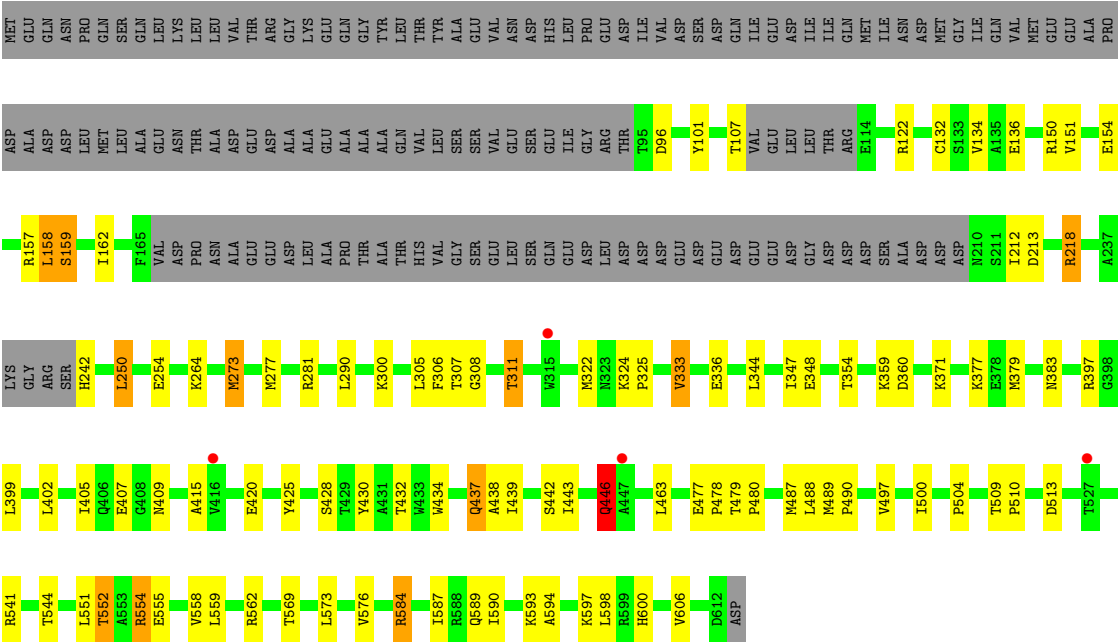








● Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.39Å 207.24Å 308.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 3.95 49.92 – 3.95	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.92-3.95) 96.1 (49.92-3.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.276 , 0.325 0.275 , 0.325	Depositor DCC
R_{free} test set	2079 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	142.5	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 228.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	49826	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/2263	0.86	6/3073 (0.2%)
1	B	0.34	0/2185	0.80	0/2967
1	G	0.32	0/1636	0.86	4/2221 (0.2%)
1	H	0.32	0/1623	0.84	2/2205 (0.1%)
2	C	0.36	0/9653	0.82	13/13062 (0.1%)
2	I	0.34	0/9676	0.82	7/13089 (0.1%)
3	D	0.41	0/7644	0.94	23/10385 (0.2%)
3	J	0.37	0/7607	0.90	17/10334 (0.2%)
4	E	0.54	0/482	1.34	5/662 (0.8%)
4	K	0.42	0/407	0.99	2/558 (0.4%)
5	F	0.34	0/3636	0.85	7/4892 (0.1%)
5	L	0.34	0/3636	0.87	10/4892 (0.2%)
All	All	0.36	0/50448	0.87	96/68340 (0.1%)

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	109	ALA	CA-C-N	14.39	137.83	119.84
2	I	109	ALA	C-N-CA	14.39	137.83	119.84
5	L	489	MET	CA-C-N	12.66	135.66	119.84
5	L	489	MET	C-N-CA	12.66	135.66	119.84
5	F	489	MET	CA-C-N	12.30	135.22	119.84
5	F	489	MET	C-N-CA	12.30	135.22	119.84
3	D	1213	GLY	CA-C-N	11.79	134.58	119.84
3	D	1213	GLY	C-N-CA	11.79	134.58	119.84
4	E	39	VAL	CA-C-N	11.25	153.99	127.00
4	E	39	VAL	C-N-CA	11.25	153.99	127.00
3	J	1149	ARG	CA-C-N	10.61	133.10	119.84
3	J	1149	ARG	C-N-CA	10.61	133.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1213	GLY	CA-C-N	10.45	132.90	119.84
3	J	1213	GLY	C-N-CA	10.45	132.90	119.84
3	D	850	LYS	CA-C-N	9.60	131.84	119.84
3	D	850	LYS	C-N-CA	9.60	131.84	119.84
4	E	36	ASP	CA-C-N	9.57	131.80	119.84
4	E	36	ASP	C-N-CA	9.57	131.80	119.84
5	L	600	HIS	CA-C-N	9.44	129.53	119.05
5	L	600	HIS	C-N-CA	9.44	129.53	119.05
3	D	1149	ARG	CA-C-N	8.88	130.94	119.84
3	D	1149	ARG	C-N-CA	8.88	130.94	119.84
3	J	858	VAL	CA-C-N	8.80	130.84	119.84
3	J	858	VAL	C-N-CA	8.80	130.84	119.84
2	C	42	ASP	CA-C-N	8.48	128.09	118.85
2	C	42	ASP	C-N-CA	8.48	128.09	118.85
3	J	1152	GLU	CA-C-N	8.39	130.32	119.84
3	J	1152	GLU	C-N-CA	8.39	130.32	119.84
1	A	10	LYS	CA-C-N	8.35	128.41	119.90
1	A	10	LYS	C-N-CA	8.35	128.41	119.90
3	J	850	LYS	CA-C-N	8.18	130.06	119.84
3	J	850	LYS	C-N-CA	8.18	130.06	119.84
3	D	1152	GLU	CA-C-N	8.12	129.99	119.84
3	D	1152	GLU	C-N-CA	8.12	129.99	119.84
1	H	29	GLU	CA-C-N	-8.03	109.80	119.84
1	H	29	GLU	C-N-CA	-8.03	109.80	119.84
1	G	29	GLU	CA-C-N	-7.94	109.92	119.84
1	G	29	GLU	C-N-CA	-7.94	109.92	119.84
2	I	566	GLY	CA-C-N	7.88	127.79	119.05
2	I	566	GLY	C-N-CA	7.88	127.79	119.05
3	D	823	THR	CA-C-N	7.45	127.16	119.56
3	D	823	THR	C-N-CA	7.45	127.16	119.56
3	D	358	GLY	CA-C-N	6.92	126.89	119.28
3	D	358	GLY	C-N-CA	6.92	126.89	119.28
3	D	246	PRO	CA-C-N	6.81	126.61	119.05
3	D	246	PRO	C-N-CA	6.81	126.61	119.05
4	E	32	VAL	N-CA-C	6.51	116.65	110.53
2	C	1204	LEU	CA-C-N	6.50	142.61	127.00
2	C	1204	LEU	C-N-CA	6.50	142.61	127.00
3	D	583	VAL	CA-C-N	-6.49	112.23	118.97
3	D	583	VAL	C-N-CA	-6.49	112.23	118.97
4	K	36	ASP	CA-C-N	6.28	127.69	119.84
4	K	36	ASP	C-N-CA	6.28	127.69	119.84
2	I	1204	LEU	CA-C-N	6.10	141.64	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1204	LEU	C-N-CA	6.10	141.64	127.00
5	F	382	ALA	N-CA-C	5.97	117.86	111.36
3	D	1315	ALA	N-CA-C	5.95	118.72	111.82
5	L	96	ASP	CA-C-N	5.89	125.76	119.28
5	L	96	ASP	C-N-CA	5.89	125.76	119.28
5	L	213	ASP	CA-C-N	5.81	127.11	119.84
5	L	213	ASP	C-N-CA	5.81	127.11	119.84
2	C	566	GLY	CA-C-N	5.81	125.50	119.05
2	C	566	GLY	C-N-CA	5.81	125.50	119.05
1	A	153	VAL	CA-C-N	5.66	125.97	119.92
1	A	153	VAL	C-N-CA	5.66	125.97	119.92
5	F	213	ASP	CA-C-N	5.65	126.90	119.84
5	F	213	ASP	C-N-CA	5.65	126.90	119.84
5	L	446	GLN	N-CA-C	5.61	118.59	111.69
1	G	178	SER	CA-C-N	5.60	125.26	119.05
1	G	178	SER	C-N-CA	5.60	125.26	119.05
2	I	105	TYR	N-CA-C	5.56	113.34	108.78
5	F	150	ARG	N-CA-C	-5.55	107.51	114.56
2	C	1316	GLU	CA-C-N	5.54	125.53	120.21
2	C	1316	GLU	C-N-CA	5.54	125.53	120.21
3	J	853	THR	CB-CA-C	-5.51	109.73	117.23
3	J	529	GLY	CA-C-N	5.43	125.25	119.28
3	J	529	GLY	C-N-CA	5.43	125.25	119.28
2	C	668	ILE	N-CA-C	5.40	112.89	107.55
3	D	240	THR	N-CA-C	-5.36	105.80	112.93
2	C	242	VAL	CA-C-N	5.36	125.43	119.32
2	C	242	VAL	C-N-CA	5.36	125.43	119.32
3	J	839	VAL	N-CA-C	5.32	116.10	110.72
5	F	244	THR	N-CA-C	-5.30	105.55	112.23
3	D	853	THR	CB-CA-C	-5.28	110.04	117.23
2	C	891	GLY	N-CA-C	-5.22	107.84	114.16
2	C	12	ARG	CB-CA-C	-5.17	110.64	116.63
5	L	150	ARG	N-CA-C	-5.16	108.01	114.56
3	D	492	SER	CA-C-N	5.09	125.17	119.87
3	D	492	SER	C-N-CA	5.09	125.17	119.87
3	J	552	ILE	N-CA-C	5.08	115.78	108.93
3	D	587	LEU	CA-C-N	-5.06	113.51	119.84
3	D	587	LEU	C-N-CA	-5.06	113.51	119.84
1	A	178	SER	CA-C-N	5.03	125.47	120.04
1	A	178	SER	C-N-CA	5.03	125.47	120.04
3	J	583	VAL	CA-C-N	-5.02	113.75	118.97
3	J	583	VAL	C-N-CA	-5.02	113.75	118.97

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	2236	0	2254	32	0
1	B	2160	0	2184	31	0
1	G	1618	0	1622	22	0
1	H	1605	0	1599	28	0
2	C	9522	0	8569	115	0
2	I	9544	0	8601	129	0
3	D	7549	0	6266	93	0
3	J	7512	0	6245	93	0
4	E	482	0	301	7	0
4	K	408	0	255	10	0
5	F	3592	0	3433	44	0
5	L	3592	0	3433	48	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	49826	0	44762	582	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 6.

All (582) 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)
3:J:910:ASN:CG	4:K:15:ASN:HB2	1.65	1.21
2:I:936:ARG:HH21	2:I:936:ARG:HG3	1.29	0.98
2:C:936:ARG:HH21	2:C:936:ARG:HG3	1.33	0.92
2:C:808:ASN:H	3:D:633:ALA:HB2	1.44	0.82
1:G:11:PRO:HA	1:G:30:PRO:HD2	1.65	0.79
2:I:185:ASP:HB2	2:I:197:ARG:HB2	1.65	0.76
5:L:218:ARG:HH11	5:L:218:ARG:HG2	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:218:ARG:HG2	5:F:218:ARG:HH11	1.50	0.75
3:J:288:PRO:HA	5:L:377:LYS:HE3	1.69	0.74
1:A:228:LEU:O	1:A:230:ALA:N	2.20	0.73
2:I:345:PRO:O	2:I:347:ILE:N	2.21	0.72
2:I:26:TYR:HB2	2:I:29:SER:HB3	1.70	0.72
3:J:317:THR:HA	3:J:323:PRO:HA	1.71	0.72
1:G:44:ARG:NH1	2:I:1087:TYR:OH	2.23	0.71
2:I:1101:LEU:HB3	3:J:731:ARG:HG3	1.73	0.70
3:J:910:ASN:CG	4:K:15:ASN:CB	2.56	0.70
2:C:345:PRO:O	2:C:347:ILE:N	2.23	0.70
1:H:71:LYS:NZ	1:H:139:SER:O	2.24	0.70
2:I:931:VAL:HB	2:I:944:ARG:HH22	1.57	0.69
4:E:26:ARG:NH1	4:E:29:GLN:OE1	2.26	0.69
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.75	0.68
3:J:910:ASN:HB2	4:K:15:ASN:HA	1.76	0.68
2:C:931:VAL:HB	2:C:944:ARG:HH22	1.58	0.67
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.77	0.67
2:C:832:HIS:HE1	2:C:1058:ARG:HB2	1.59	0.67
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.27	0.67
1:G:230:ALA:O	1:G:232:VAL:N	2.28	0.67
5:F:276:MET:SD	5:F:279:ARG:NH2	2.69	0.66
2:C:408:SER:O	2:C:431:LYS:NZ	2.28	0.66
5:F:397:ARG:HG2	5:F:443:ILE:HD12	1.77	0.65
2:I:147:SER:HB2	2:I:530:ILE:HG22	1.78	0.65
5:L:399:LEU:HD13	5:L:446:GLN:HG2	1.79	0.65
2:C:404:LYS:HE2	2:C:586:PHE:HZ	1.62	0.65
3:J:114:ILE:HD11	3:J:307:LEU:HB2	1.79	0.65
1:G:66:HIS:HB3	2:I:874:GLY:HA2	1.78	0.65
3:D:102:MET:HG2	3:D:246:PRO:HD3	1.79	0.64
3:J:245:LEU:O	3:J:250:ARG:NH1	2.30	0.64
1:A:208:ASN:OD1	1:A:210:THR:OG1	2.13	0.64
1:H:11:PRO:HA	1:H:30:PRO:HD2	1.80	0.64
1:H:78:ILE:HD13	1:H:81:ILE:HD12	1.79	0.64
5:F:587:ILE:HD12	5:F:590:ILE:HD11	1.79	0.64
5:L:428:SER:O	5:L:432:THR:OG1	2.14	0.63
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.81	0.63
2:C:979:LEU:HD21	2:C:1000:LEU:HD23	1.81	0.63
3:J:901:ARG:O	3:J:1251:LYS:NZ	2.32	0.63
5:L:151:VAL:HG11	5:L:158:LEU:HG	1.81	0.62
1:B:110:VAL:HG21	1:B:140:ILE:HD11	1.80	0.62
2:C:890:LYS:HG2	2:C:914:LYS:HB2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:548:ARG:NH2	2:C:567:PRO:O	2.33	0.62
5:L:587:ILE:HD12	5:L:590:ILE:HD11	1.82	0.62
2:C:148:GLN:NE2	2:C:533:LEU:O	2.29	0.61
1:A:110:VAL:HG21	1:A:140:ILE:HD11	1.82	0.61
2:C:56:VAL:HG21	2:C:468:LEU:HB3	1.81	0.61
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.35	0.61
2:I:898:GLU:HG2	5:L:541:ARG:HA	1.83	0.61
2:C:222:ASP:OD1	2:C:227:LYS:NZ	2.28	0.61
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.82	0.61
2:I:74:ARG:NE	2:I:121:GLU:OE2	2.32	0.61
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.83	0.60
3:J:821:MET:HA	3:J:881:LYS:HA	1.82	0.60
5:L:551:LEU:HD11	5:L:555:GLU:HG3	1.84	0.60
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.84	0.60
1:A:150:ARG:HE	1:B:6:THR:HA	1.65	0.60
2:C:189:ASP:OD1	2:C:193:ASN:N	2.34	0.60
3:D:452:LEU:HG	3:D:625:MET:HE3	1.82	0.60
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.84	0.60
5:F:590:ILE:HA	5:F:593:LYS:HG2	1.82	0.60
2:I:915:ASP:OD2	2:I:919:ARG:NH2	2.34	0.60
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.85	0.59
3:D:693:VAL:HG21	3:D:743:MET:HG3	1.84	0.59
1:H:100:LEU:HD21	1:H:121:VAL:HG21	1.85	0.59
3:D:491:LEU:HA	3:D:499:ILE:H	1.68	0.58
2:C:703:GLY:N	2:C:705:GLU:OE2	2.37	0.58
3:D:506:VAL:HG13	3:D:628:GLY:HA3	1.85	0.58
2:C:152:SER:OG	2:C:452:ARG:HG2	2.04	0.58
3:D:288:PRO:HA	5:F:377:LYS:HE3	1.84	0.58
2:I:548:ARG:NH2	2:I:567:PRO:O	2.37	0.58
2:I:808:ASN:H	3:J:633:ALA:HB2	1.68	0.58
2:C:1209:GLN:HA	2:C:1226:THR:HA	1.85	0.58
5:F:213:ASP:OD1	5:F:213:ASP:N	2.33	0.58
3:D:271:ARG:NH1	5:F:400:GLN:OE1	2.38	0.57
1:H:102:LEU:HG	1:H:115:ILE:HG12	1.84	0.57
5:L:590:ILE:HA	5:L:593:LYS:HG2	1.85	0.57
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.85	0.57
2:I:1209:GLN:HA	2:I:1226:THR:HA	1.86	0.57
1:G:110:VAL:HG21	1:G:140:ILE:HD11	1.85	0.57
3:D:746:LEU:HD22	3:D:758:PRO:HB3	1.86	0.57
2:C:21:VAL:HG21	2:C:592:ARG:HD3	1.85	0.57
1:G:71:LYS:NZ	1:G:139:SER:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:HIS:CE1	2:C:454:ARG:HD2	2.40	0.57
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.87	0.57
5:L:277:MET:HE3	5:L:281:ARG:HG3	1.87	0.57
3:J:118:LYS:HE3	3:J:312:ARG:HG2	1.87	0.57
2:C:1099:ASN:ND2	3:D:505:ASP:OD2	2.36	0.56
1:B:37:HIS:CE1	1:B:187:VAL:HG21	2.39	0.56
2:C:915:ASP:OD2	2:C:919:ARG:NH2	2.37	0.56
2:C:1289:GLU:HB3	2:C:1294:LYS:HD2	1.87	0.56
2:I:222:ASP:OD1	2:I:227:LYS:NZ	2.39	0.56
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.87	0.55
1:A:285:THR:HG23	1:A:288:GLU:H	1.71	0.55
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.36	0.55
3:D:108:ALA:HB3	3:D:279:LEU:HD23	1.88	0.55
3:D:210:SER:O	3:D:214:ARG:NH2	2.40	0.55
2:I:887:VAL:HB	2:I:913:VAL:HB	1.88	0.55
2:I:936:ARG:HG3	2:I:936:ARG:NH2	2.05	0.55
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.40	0.55
2:I:21:VAL:HG21	2:I:592:ARG:HD3	1.89	0.55
2:C:314:ASN:O	2:C:352:ARG:NH2	2.41	0.54
5:F:120:ALA:HB1	5:F:421:TYR:HB2	1.88	0.54
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.88	0.54
3:J:481:ARG:HA	3:J:485:MET:HG2	1.89	0.54
3:J:527:LEU:O	3:J:529:GLY:N	2.39	0.54
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.42	0.54
1:B:182:ARG:HD3	3:D:531:LYS:HA	1.90	0.54
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.89	0.54
2:C:1101:LEU:HB3	3:D:731:ARG:HG3	1.90	0.54
2:C:1153:ALA:O	2:C:1155:VAL:N	2.41	0.54
1:G:78:ILE:HD13	1:G:81:ILE:HD12	1.88	0.54
2:I:960:LEU:HD22	2:I:1029:LEU:HD12	1.89	0.54
1:A:102:LEU:HG	1:A:115:ILE:HG12	1.89	0.54
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.87	0.54
5:L:551:LEU:HD22	5:L:552:THR:H	1.73	0.54
1:H:91:ARG:NH2	1:H:210:THR:O	2.40	0.54
1:A:75:GLN:HE21	2:C:727:VAL:HG11	1.71	0.53
2:C:960:LEU:HD22	2:C:1029:LEU:HG	1.90	0.53
3:D:813:ASP:OD1	3:D:883:ARG:NH2	2.37	0.53
5:F:151:VAL:HG11	5:F:158:LEU:HG	1.90	0.53
5:L:101:TYR:CE2	5:L:405:ILE:HD13	2.43	0.53
2:C:316:GLU:HG3	2:C:352:ARG:NH2	2.23	0.53
3:D:609:TYR:HA	3:D:617:THR:OG1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:232:ASN:N	3:D:232:ASN:OD1	2.40	0.53
2:C:246:LEU:HB3	2:C:269:ILE:HD13	1.90	0.53
2:C:936:ARG:HG3	2:C:936:ARG:NH2	2.10	0.53
3:D:364:HIS:HB2	3:D:485:MET:HE1	1.91	0.53
5:F:97:PRO:HB2	5:F:402:LEU:HD21	1.91	0.53
3:J:232:ASN:OD1	3:J:232:ASN:N	2.39	0.53
3:D:245:LEU:O	3:D:250:ARG:NH1	2.41	0.53
2:I:150:HIS:CE1	2:I:454:ARG:HD2	2.44	0.53
2:I:228:VAL:HG23	2:I:337:PHE:HB2	1.90	0.53
5:L:277:MET:HE1	5:L:359:LYS:HG2	1.90	0.53
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.89	0.53
2:I:86:GLN:HA	2:I:140:GLY:HA2	1.89	0.53
1:A:78:ILE:HD13	1:A:81:ILE:HD12	1.90	0.53
2:I:1075:VAL:HG21	3:J:354:VAL:HG11	1.90	0.53
5:L:573:LEU:HD13	5:L:584:ARG:HE	1.73	0.53
1:B:184:ALA:HB3	1:B:204:GLU:HB3	1.90	0.52
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.91	0.52
2:I:237:LEU:HD13	2:I:292:ILE:HD12	1.91	0.52
2:I:798:GLN:OE1	2:I:828:PHE:N	2.35	0.52
3:J:353:SER:HB3	3:J:447:ILE:HG13	1.91	0.52
2:I:979:LEU:HD21	2:I:1000:LEU:HD23	1.91	0.52
2:I:1276:TRP:CE2	3:J:801:VAL:HG11	2.44	0.52
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.20	0.52
5:L:134:VAL:HG22	5:L:273:MET:HE1	1.90	0.52
1:B:12:ARG:HG3	1:B:30:PRO:HG3	1.91	0.52
1:B:16:ILE:HG12	1:B:26:VAL:HG22	1.92	0.52
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.92	0.52
3:D:1168:GLU:O	3:D:1170:LYS:N	2.42	0.52
1:G:91:ARG:NH2	1:G:209:GLY:O	2.43	0.52
2:I:1244:HIS:HB2	2:I:1265:PHE:CG	2.45	0.52
3:D:179:LYS:O	3:D:184:ALA:HB2	2.10	0.52
3:D:471:PRO:O	3:D:477:GLN:NE2	2.43	0.52
1:H:110:VAL:HG21	1:H:140:ILE:HD11	1.91	0.52
2:I:933:VAL:HG13	2:I:1050:VAL:HG22	1.92	0.52
2:C:1154:ASP:O	2:C:1156:ARG:N	2.43	0.52
2:I:836:LEU:HB3	2:I:918:LEU:HD21	1.92	0.52
2:I:811:ASN:HB2	2:I:1099:ASN:HB2	1.90	0.52
3:D:1169:THR:HA	3:D:1174:ARG:HA	1.91	0.51
5:F:278:ASP:OD1	5:F:281:ARG:NH2	2.43	0.51
1:A:282:VAL:HB	1:A:316:MET:HB2	1.92	0.51
1:B:212:ASP:HB2	1:B:215:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:785:ASP:OD2	2:C:791:LEU:N	2.42	0.51
1:G:182:ARG:NH1	2:I:1092:THR:OG1	2.42	0.51
3:J:48:THR:HG22	3:J:50:LYS:HG2	1.92	0.51
4:K:13:ILE:HG22	4:K:14:GLY:N	2.25	0.51
3:D:690:ASN:ND2	3:D:743:MET:SD	2.83	0.51
5:F:277:MET:HE3	5:F:281:ARG:HG3	1.93	0.51
3:J:274:ASN:ND2	5:L:446:GLN:OE1	2.43	0.51
2:C:48:GLY:C	2:C:50:GLU:H	2.18	0.51
4:E:15:ASN:O	4:E:17:PHE:N	2.43	0.51
1:H:180:VAL:HG11	1:H:183:ILE:HD11	1.92	0.51
1:H:184:ALA:HB3	1:H:204:GLU:HB3	1.91	0.51
2:I:344:GLY:H	2:I:437:ASN:HD21	1.59	0.51
1:H:179:PRO:HB3	1:H:211:ILE:HG23	1.92	0.51
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.93	0.51
2:C:1070:HIS:NE2	2:C:1114:GLU:OE2	2.44	0.51
5:F:95:THR:OG1	5:F:96:ASP:N	2.38	0.51
1:H:37:HIS:CE1	1:H:187:VAL:HG21	2.45	0.51
2:C:1065:LYS:HE2	2:C:1235:LEU:HD12	1.92	0.51
2:I:796:LEU:N	2:I:1231:TYR:OH	2.44	0.51
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.93	0.51
5:L:218:ARG:HH11	5:L:218:ARG:CG	2.22	0.51
1:B:41:ASN:HD21	2:C:1217:THR:HG22	1.75	0.51
3:D:1257:VAL:HA	3:D:1260:MET:HE3	1.93	0.51
3:J:46:TYR:CZ	3:J:47:ARG:HG3	2.45	0.50
2:C:548:ARG:O	3:D:780:ARG:NH1	2.45	0.50
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.11	0.50
2:I:227:LYS:NZ	2:I:334:GLU:OE2	2.35	0.50
1:A:52:PRO:HG3	1:A:150:ARG:NH1	2.26	0.50
3:D:294:ASN:HD22	5:F:406:GLN:HE21	1.59	0.50
3:D:865:HIS:HB3	3:D:868:TRP:HD1	1.76	0.50
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.94	0.50
3:D:461:PHE:C	3:D:463:GLY:H	2.20	0.50
4:K:13:ILE:CG1	4:K:19:LEU:HD13	2.41	0.50
2:C:1101:LEU:HD22	3:D:731:ARG:HB2	1.93	0.50
2:I:890:LYS:HG2	2:I:914:LYS:HE3	1.94	0.50
1:A:71:LYS:NZ	1:A:139:SER:O	2.45	0.50
2:C:300:ASP:OD1	2:C:313:ALA:N	2.43	0.50
1:B:71:LYS:NZ	1:B:139:SER:O	2.45	0.49
2:C:796:LEU:N	2:C:1231:TYR:OH	2.45	0.49
4:E:79:GLU:O	4:E:81:GLN:N	2.44	0.49
3:D:140:TYR:HD1	3:D:297:ARG:HD3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:338:THR:HB	2:I:345:PRO:HD3	1.93	0.49
2:I:785:ASP:OD2	2:I:791:LEU:N	2.44	0.49
2:I:1268:GLN:NE2	3:J:352:ARG:HB3	2.27	0.49
3:D:370:LYS:HB3	3:D:409:TRP:CZ3	2.47	0.49
2:C:1226:THR:HG23	3:D:638:SER:OG	2.13	0.49
5:F:218:ARG:HH11	5:F:218:ARG:CG	2.22	0.49
2:I:404:LYS:HE2	2:I:586:PHE:HZ	1.77	0.49
5:L:122:ARG:HG2	5:L:371:LYS:HE2	1.94	0.49
3:D:57:PHE:O	3:D:98:ARG:NH2	2.46	0.49
1:H:66:HIS:HD2	1:H:68:TYR:HB3	1.77	0.49
3:D:46:TYR:CZ	3:D:47:ARG:HG3	2.48	0.49
5:F:303:ILE:O	5:F:307:THR:OG1	2.21	0.49
1:H:42:ALA:O	1:H:46:ILE:HG12	2.13	0.49
2:I:338:THR:HG21	2:I:345:PRO:HB3	1.95	0.49
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.13	0.49
2:C:404:LYS:HE2	2:C:586:PHE:CZ	2.47	0.49
2:C:562:GLU:OE1	2:C:662:SER:OG	2.24	0.49
1:A:44:ARG:HG3	1:A:183:ILE:HB	1.95	0.48
3:J:102:MET:HG2	3:J:246:PRO:HD3	1.94	0.48
2:C:344:GLY:H	2:C:437:ASN:HD21	1.61	0.48
3:J:865:HIS:H	3:J:868:TRP:HB2	1.78	0.48
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.96	0.48
2:I:1243:MET:SD	3:J:445:LYS:HB3	2.53	0.48
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.96	0.48
3:D:1318:SER:HB2	3:D:1342:ASP:OD2	2.13	0.48
1:G:182:ARG:HD2	2:I:1092:THR:HA	1.94	0.48
2:I:90:VAL:HG11	2:I:1035:LYS:HZ1	1.78	0.48
2:C:903:ARG:O	2:C:907:GLY:N	2.46	0.48
2:I:530:ILE:HG12	2:I:573:ASN:O	2.14	0.48
1:B:196:THR:OG1	1:B:197:ASP:OD1	2.31	0.48
2:C:26:TYR:HB2	2:C:29:SER:HB3	1.95	0.48
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.11	0.48
2:I:629:PHE:CE2	2:I:634:VAL:HG12	2.49	0.48
1:B:285:THR:HG23	1:B:288:GLU:H	1.79	0.48
3:J:108:ALA:HB3	3:J:279:LEU:HD23	1.96	0.48
1:B:91:ARG:NH2	1:B:210:THR:O	2.46	0.48
2:C:67:GLU:O	2:C:102:LEU:HD12	2.14	0.48
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.28	0.48
2:C:832:HIS:CE1	2:C:1058:ARG:HB2	2.45	0.48
2:I:180:ARG:NH2	2:I:392:GLU:O	2.46	0.48
2:I:717:VAL:HG12	2:I:782:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1255:THR:HB	2:I:1257:GLN:HG3	1.94	0.48
2:I:701:GLY:O	2:I:1184:THR:N	2.33	0.48
2:C:1177:ARG:C	2:C:1179:GLY:H	2.22	0.48
1:B:37:HIS:CD2	2:C:1216:ARG:HG2	2.49	0.47
2:C:626:GLU:HA	2:C:627:GLY:C	2.39	0.47
4:E:16:ARG:O	4:E:19:LEU:HB3	2.14	0.47
3:J:747:MET:HE2	3:J:775:SER:HA	1.96	0.47
3:D:733:SER:O	3:D:737:ILE:HG12	2.14	0.47
3:J:210:SER:O	3:J:214:ARG:NH2	2.46	0.47
5:L:439:ILE:O	5:L:443:ILE:HG13	2.15	0.47
3:D:1295:ASN:O	3:J:1225:GLY:HA3	2.13	0.47
2:I:703:GLY:N	2:I:705:GLU:OE2	2.46	0.47
2:I:1294:LYS:O	3:J:348:ASP:N	2.33	0.47
1:A:134:THR:HG21	2:C:727:VAL:O	2.15	0.47
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.47	0.47
2:I:160:ASP:C	2:I:162:GLY:H	2.23	0.47
3:J:452:LEU:HG	3:J:625:MET:HE3	1.97	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.74	0.47
1:B:37:HIS:CG	2:C:1216:ARG:HG2	2.49	0.47
3:J:739:GLN:HE21	3:J:744:ARG:HG3	1.79	0.47
1:A:133:LEU:HD21	1:A:140:ILE:HG12	1.97	0.47
3:J:690:ASN:ND2	3:J:743:MET:SD	2.88	0.47
5:F:399:LEU:HD23	5:F:443:ILE:HG22	1.97	0.47
1:B:180:VAL:HA	1:B:207:THR:HA	1.97	0.47
3:D:650:LYS:NZ	3:D:765:GLU:OE2	2.39	0.47
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.50	0.47
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.96	0.47
2:C:151:ARG:HH21	2:C:445:ILE:HG21	1.80	0.46
2:C:344:GLY:H	2:C:437:ASN:ND2	2.12	0.46
3:D:550:VAL:O	3:D:569:LEU:HA	2.15	0.46
3:J:260:PHE:HB3	5:L:504:PRO:HB3	1.98	0.46
3:D:317:THR:HA	3:D:323:PRO:HA	1.96	0.46
2:I:805:MET:HE1	2:I:1221:PHE:CE1	2.50	0.46
3:J:647:PRO:HG3	3:J:697:MET:HA	1.96	0.46
5:L:463:LEU:HD13	5:L:487:MET:SD	2.55	0.46
3:J:127:LEU:HD23	3:J:127:LEU:HA	1.71	0.46
3:J:556:GLU:O	3:J:558:ASP:N	2.48	0.46
1:B:78:ILE:HD13	1:B:81:ILE:HD12	1.98	0.46
5:F:520:GLY:HA2	5:F:523:ILE:HD12	1.97	0.46
1:G:59:VAL:HG21	1:G:85:LEU:HD13	1.97	0.46
1:G:76:GLU:CD	1:G:76:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:THR:HB	1:A:207:THR:O	2.16	0.46
1:H:82:LEU:O	1:H:86:LYS:HG3	2.15	0.46
5:L:555:GLU:HB2	5:L:594:ALA:HB2	1.97	0.46
1:A:224:LEU:O	1:A:228:LEU:HG	2.16	0.46
2:I:367:TYR:CD1	2:I:376:PRO:HB3	2.51	0.46
2:I:1101:LEU:HD22	3:J:731:ARG:HB2	1.98	0.46
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.97	0.46
3:D:603:LYS:O	3:D:607:THR:OG1	2.34	0.46
1:H:180:VAL:HA	1:H:207:THR:HA	1.97	0.46
2:I:1186:VAL:HG13	2:I:1187:PHE:HD2	1.81	0.46
3:J:419:HIS:O	3:J:439:PRO:HD2	2.15	0.46
5:L:487:MET:HA	5:L:487:MET:HE2	1.98	0.46
2:C:848:GLU:HG2	2:C:888:THR:HA	1.98	0.46
5:F:487:MET:HE2	5:F:487:MET:HA	1.97	0.46
2:I:300:ASP:OD1	2:I:313:ALA:N	2.43	0.46
2:I:1099:ASN:ND2	3:J:505:ASP:OD2	2.49	0.46
3:J:615:LYS:H	4:K:7:GLN:CG	2.29	0.46
1:A:27:THR:HG22	1:A:202:VAL:HG13	1.97	0.46
1:B:195:ARG:O	1:B:197:ASP:N	2.43	0.46
2:C:48:GLY:O	2:C:50:GLU:N	2.39	0.46
2:I:144:VAL:HG23	2:I:515:MET:HG2	1.97	0.46
3:J:269:TYR:O	3:J:273:ILE:HG13	2.16	0.46
3:J:738:ARG:O	3:J:742:GLY:N	2.48	0.46
5:L:157:ARG:HG3	5:L:159:SER:H	1.80	0.46
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.16	0.45
3:D:842:ARG:HD2	3:D:842:ARG:HA	1.61	0.45
5:F:134:VAL:HG22	5:F:273:MET:HE1	1.98	0.45
1:G:37:HIS:CE1	1:G:187:VAL:HG21	2.51	0.45
3:J:425:ARG:HB2	3:J:466:MET:HG2	1.98	0.45
5:L:407:GLU:HG3	5:L:442:SER:OG	2.16	0.45
5:L:562:ARG:HG2	5:L:576:VAL:HG21	1.99	0.45
2:I:225:PHE:CE1	2:I:345:PRO:HA	2.51	0.45
3:J:262:THR:HG22	5:L:504:PRO:HB2	1.98	0.45
1:A:42:ALA:O	1:A:46:ILE:HG12	2.15	0.45
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.51	0.45
2:I:819:SER:HA	2:I:1085:MET:HE3	1.98	0.45
2:C:812:PHE:HB3	3:D:357:VAL:HG21	1.98	0.45
3:J:35:PHE:CD2	3:J:101:ARG:HD3	2.52	0.45
3:J:1160:SER:O	3:J:1162:ILE:N	2.50	0.45
3:D:425:ARG:HB2	3:D:466:MET:HG2	1.97	0.45
5:F:608:ARG:C	5:F:610:PHE:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:305:LEU:HD11	5:L:322:MET:HE1	1.99	0.45
2:C:728:ASP:HB3	2:C:731:ARG:H	1.82	0.45
3:D:739:GLN:HG3	3:D:744:ARG:HG3	1.97	0.45
1:H:56:VAL:HG12	1:H:173:VAL:HG11	1.99	0.45
3:D:262:THR:HG22	5:F:504:PRO:HB2	1.98	0.45
5:F:343:LYS:O	5:F:347:ILE:HG13	2.17	0.45
2:I:206:ALA:O	2:I:209:ILE:HG22	2.16	0.45
2:I:663:VAL:O	2:I:666:SER:HB2	2.17	0.45
3:D:678:ARG:NH2	3:D:756:GLU:OE1	2.48	0.45
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.99	0.45
1:A:37:HIS:CE1	1:A:187:VAL:HG21	2.51	0.45
1:A:59:VAL:HG21	1:A:85:LEU:HD13	1.98	0.45
2:C:92:TYR:CE2	2:C:129:LEU:HB2	2.51	0.45
2:I:225:PHE:HE1	2:I:345:PRO:HA	1.81	0.45
2:C:1221:PHE:HD1	3:D:634:ARG:HA	1.82	0.44
2:I:1087:TYR:CZ	2:I:1213:TYR:HB2	2.52	0.44
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.48	0.44
3:J:842:ARG:HD2	3:J:842:ARG:HA	1.57	0.44
2:C:391:SER:OG	2:C:393:ASP:OD1	2.32	0.44
2:I:127:ILE:HA	2:I:128:PRO:HD3	1.86	0.44
5:L:250:LEU:O	5:L:254:GLU:HG2	2.18	0.44
5:L:379:MET:O	5:L:383:ASN:ND2	2.50	0.44
2:I:682:GLY:O	2:I:686:GLN:HG3	2.17	0.44
3:J:847:ASP:HA	3:J:860:ARG:HB2	1.99	0.44
1:B:66:HIS:HD2	1:B:68:TYR:H	1.66	0.44
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.98	0.44
1:H:51:MET:HA	1:H:52:PRO:HD3	1.76	0.44
2:I:1333:LEU:HD13	3:J:115:TRP:CZ3	2.52	0.44
3:J:376:LEU:HB3	3:J:470:VAL:HG21	2.00	0.44
2:C:228:VAL:HG23	2:C:337:PHE:HB2	2.00	0.44
4:E:26:ARG:HH21	4:E:37:PRO:CB	2.30	0.44
1:G:134:THR:HG21	2:I:727:VAL:O	2.18	0.44
1:H:41:ASN:ND2	2:I:1217:THR:HG22	2.32	0.44
2:I:1226:THR:HG23	3:J:638:SER:OG	2.18	0.44
3:J:190:LYS:HG3	3:J:235:GLU:CD	2.42	0.44
5:L:290:LEU:HB3	5:L:333:VAL:HG21	2.00	0.44
1:B:273:GLU:OE2	1:B:293:PRO:HD2	2.17	0.44
2:C:645:PHE:CG	2:C:649:GLN:HB2	2.52	0.44
3:D:451:PRO:HB2	3:D:625:MET:HE2	1.99	0.44
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.17	0.44
5:L:344:LEU:HD12	5:L:347:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.99	0.44
3:J:746:LEU:HD22	3:J:758:PRO:HB3	1.99	0.44
3:D:496:GLY:HA3	3:D:903:LEU:HD22	2.00	0.44
5:F:277:MET:HE1	5:F:359:LYS:HG2	2.00	0.44
2:I:344:GLY:H	2:I:437:ASN:ND2	2.16	0.44
2:I:1336:ASN:HA	3:J:33:TRP:HH2	1.83	0.44
3:J:114:ILE:H	3:J:114:ILE:HG13	1.41	0.44
3:J:857:LEU:HA	3:J:858:VAL:HA	1.57	0.44
2:C:241:LEU:HD22	2:C:285:ILE:HD13	2.00	0.44
1:G:100:LEU:HD21	1:G:121:VAL:HG21	1.99	0.44
2:I:61:SER:OG	2:I:62:TYR:N	2.51	0.44
2:I:152:SER:OG	2:I:452:ARG:HG2	2.18	0.44
2:I:363:LEU:HB3	2:I:381:ALA:HB1	2.00	0.44
2:I:685:MET:SD	2:I:1073:LYS:HD3	2.57	0.44
3:J:893:GLY:O	3:J:1258:ARG:NH2	2.45	0.44
2:I:716:ALA:HB3	2:I:784:ALA:HB3	1.99	0.43
5:L:101:TYR:OH	5:L:409:ASN:ND2	2.48	0.43
3:J:38:VAL:HG11	3:J:56:LEU:HD23	2.00	0.43
1:B:107:ILE:HG13	1:B:136:GLU:HG3	2.00	0.43
5:F:354:THR:HG22	5:F:357:GLN:HE21	1.83	0.43
1:A:91:ARG:NH2	1:A:209:GLY:O	2.51	0.43
2:C:1226:THR:HG21	3:D:639:VAL:C	2.44	0.43
1:H:86:LYS:HG2	1:H:173:VAL:HG23	2.00	0.43
2:I:575:LEU:HG	2:I:579:ALA:HB3	2.00	0.43
3:J:118:LYS:HD2	3:J:118:LYS:HA	1.62	0.43
3:J:298:MET:HG2	5:L:402:LEU:HD23	2.00	0.43
3:J:1257:VAL:HA	3:J:1260:MET:HE3	2.00	0.43
3:D:24:LEU:HD23	3:D:24:LEU:HA	1.91	0.43
5:F:270:VAL:HA	5:F:273:MET:HG3	2.00	0.43
1:G:17:GLU:HB3	1:G:25:LYS:HB2	2.00	0.43
3:J:493:PRO:HG3	3:J:904:ALA:HB2	2.00	0.43
1:B:95:LYS:NZ	1:B:96:ASP:H	2.16	0.43
2:I:637:ARG:HG3	2:I:641:GLU:O	2.19	0.43
3:J:264:ASP:HB3	3:J:324:LEU:HB3	2.01	0.43
3:D:127:LEU:HD11	3:D:227:PHE:CZ	2.54	0.43
3:D:422:LEU:HD13	3:D:484:MET:HE1	1.99	0.43
1:G:41:ASN:HD22	1:G:44:ARG:CZ	2.32	0.43
2:I:1070:HIS:NE2	2:I:1114:GLU:OE2	2.42	0.43
2:I:1297:ASP:OD1	2:I:1299:ASN:N	2.52	0.43
3:D:38:VAL:HG11	3:D:56:LEU:HD23	2.00	0.43
3:D:811:GLU:OE2	3:D:890:THR:OG1	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:555:GLU:HB2	5:F:594:ALA:HB2	2.01	0.43
2:I:189:ASP:OD1	2:I:193:ASN:N	2.51	0.43
2:I:264:GLU:HB2	2:I:267:ARG:HG3	2.01	0.43
3:J:361:LEU:HD13	3:J:366:CYS:HA	2.01	0.43
2:I:975:ILE:HD11	2:I:997:TRP:HE3	1.84	0.43
3:J:461:PHE:C	3:J:463:GLY:H	2.26	0.43
1:B:56:VAL:HG12	1:B:173:VAL:HG11	2.00	0.42
3:D:113:HIS:CD2	3:D:115:TRP:HB2	2.54	0.42
5:F:409:ASN:O	5:F:413:MET:HG3	2.18	0.42
2:I:15:PHE:HD1	2:I:15:PHE:HA	1.69	0.42
3:J:1332:LEU:HD23	3:J:1332:LEU:HA	1.89	0.42
5:L:551:LEU:CD1	5:L:555:GLU:HG3	2.47	0.42
1:A:178:SER:HA	1:A:179:PRO:HD3	1.73	0.42
3:D:353:SER:HB3	3:D:447:ILE:HG13	2.01	0.42
3:D:686:TRP:CD2	3:D:758:PRO:HG3	2.53	0.42
2:I:56:VAL:HG21	2:I:468:LEU:HB3	2.00	0.42
2:C:623:LEU:HD21	2:C:653:MET:HE1	2.01	0.42
2:C:810:TYR:CE1	2:C:1078:LYS:HD3	2.54	0.42
5:F:132:CYS:O	5:F:136:GLU:HG3	2.20	0.42
5:L:306:PHE:O	5:L:308:GLY:N	2.52	0.42
2:C:155:VAL:HG12	2:C:405:PHE:HA	2.01	0.42
2:C:255:ILE:HB	2:C:263:VAL:HB	2.01	0.42
3:D:101:ARG:O	3:D:246:PRO:HG3	2.19	0.42
2:I:150:HIS:CE1	2:I:152:SER:HA	2.54	0.42
2:I:944:ARG:HH21	2:I:1050:VAL:HG13	1.83	0.42
4:K:13:ILE:CG2	4:K:14:GLY:N	2.83	0.42
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.75	0.42
2:I:40:GLU:O	2:I:73:TYR:OH	2.34	0.42
2:I:246:LEU:HB3	2:I:269:ILE:HD13	2.01	0.42
5:L:300:LYS:HB3	5:L:300:LYS:HE3	1.81	0.42
3:D:865:HIS:H	3:D:868:TRP:HB2	1.84	0.42
1:H:76:GLU:HB2	1:H:80:GLU:HB2	2.01	0.42
3:J:212:THR:O	3:J:216:LYS:HG2	2.20	0.42
5:L:554:ARG:O	5:L:558:VAL:HG23	2.19	0.42
1:A:76:GLU:H	1:A:76:GLU:CD	2.28	0.42
2:C:338:THR:HG21	2:C:345:PRO:HB3	2.01	0.42
3:D:298:MET:HG2	5:F:402:LEU:HD23	2.02	0.42
2:I:302:ILE:HG22	2:I:309:LEU:HA	2.02	0.42
2:I:890:LYS:HE2	2:I:914:LYS:HG3	2.01	0.42
3:J:646:ILE:HA	3:J:647:PRO:HD3	1.81	0.42
1:A:29:GLU:HB3	1:A:30:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:250:ARG:O	3:D:266:ASN:ND2	2.39	0.42
3:D:1221:LEU:HD22	3:D:1306:LEU:HB2	2.02	0.42
3:D:1225:GLY:HA3	3:J:1295:ASN:O	2.20	0.42
2:I:797:GLY:N	2:I:1231:TYR:OH	2.50	0.42
2:I:905:ILE:HD11	5:L:598:LEU:HD13	2.02	0.42
2:I:1257:GLN:HG2	2:I:1296:ASP:HB3	2.02	0.42
1:B:321:TRP:HA	1:B:322:PRO:HA	1.68	0.42
2:C:38:PHE:HA	2:C:48:GLY:HA2	2.02	0.42
3:D:127:LEU:HD12	3:D:237:MET:HE1	2.01	0.42
3:D:632:ALA:O	3:D:635:SER:OG	2.38	0.42
5:F:306:PHE:O	5:F:308:GLY:N	2.53	0.42
1:H:51:MET:HB3	1:H:179:PRO:HD2	2.00	0.42
5:L:430:TYR:O	5:L:434:TRP:HD1	2.02	0.42
2:C:1253:LEU:HA	5:F:525:ASP:HB2	2.01	0.42
1:G:14:VAL:HB	1:G:29:GLU:HB2	2.02	0.42
1:H:118:ASP:HB3	1:H:121:VAL:HB	2.02	0.42
2:I:1289:GLU:HB3	2:I:1294:LYS:HD2	2.02	0.42
3:J:686:TRP:CD2	3:J:758:PRO:HG3	2.55	0.42
5:L:132:CYS:O	5:L:136:GLU:HG3	2.20	0.42
1:A:14:VAL:HB	1:A:29:GLU:HB2	2.01	0.41
3:D:779:ALA:O	3:D:783:LEU:HD22	2.20	0.41
2:I:1192:GLU:OE1	3:J:764:ARG:NH1	2.53	0.41
2:I:1251:TYR:HE1	2:I:1258:PRO:HG3	1.85	0.41
2:C:524:ILE:O	2:C:528:ARG:HG3	2.20	0.41
2:C:1121:ALA:HB1	2:C:1180:MET:HB3	2.02	0.41
5:F:300:LYS:HB3	5:F:300:LYS:HE3	1.81	0.41
2:I:1334:GLY:O	3:J:25:ALA:HB3	2.20	0.41
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.88	0.41
2:C:1083:GLU:HG2	2:C:1084:ASP:OD1	2.20	0.41
5:F:305:LEU:HD21	5:F:322:MET:HE1	2.02	0.41
2:I:906:PHE:HB3	2:I:907:GLY:H	1.54	0.41
2:I:1282:GLY:O	3:J:1361:THR:HG23	2.20	0.41
2:C:962:GLU:O	2:C:966:ILE:HG13	2.20	0.41
2:C:1191:LYS:HB2	2:C:1191:LYS:NZ	2.36	0.41
2:I:1212:LEU:HB3	2:I:1221:PHE:HD2	1.85	0.41
5:L:437:GLN:HG3	5:L:438:ALA:N	2.34	0.41
1:A:150:ARG:HH21	1:B:6:THR:CB	2.34	0.41
2:C:1022:LYS:O	2:C:1026:GLU:HG3	2.20	0.41
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.02	0.41
5:F:355:ILE:H	5:F:355:ILE:HG13	1.52	0.41
1:H:52:PRO:HG3	1:H:150:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:35:PHE:HD2	3:J:101:ARG:HD3	1.84	0.41
1:A:51:MET:HA	1:A:52:PRO:HD3	1.69	0.41
2:C:218:GLU:HG2	2:C:299:LYS:HA	2.01	0.41
2:C:1199:LEU:O	2:C:1204:LEU:N	2.44	0.41
2:C:1336:ASN:N	3:D:23:ALA:O	2.54	0.41
2:I:1022:LYS:O	2:I:1026:GLU:HG3	2.21	0.41
2:I:1118:GLY:HA3	2:I:1229:TYR:O	2.20	0.41
3:J:69:GLU:HG3	3:J:76:LYS:HG2	2.02	0.41
3:J:187:ALA:O	3:J:191:SER:HB2	2.21	0.41
5:L:477:GLU:HA	5:L:478:PRO:HD3	1.81	0.41
1:A:282:VAL:O	1:A:316:MET:N	2.45	0.41
2:C:697:LYS:O	2:C:799:ASN:ND2	2.49	0.41
3:D:278:ARG:HD3	5:F:406:GLN:HB3	2.02	0.41
3:D:1360:GLY:HA2	4:E:17:PHE:CD2	2.55	0.41
5:F:216:LEU:O	5:F:219:GLU:HB3	2.21	0.41
1:G:42:ALA:O	1:G:46:ILE:HG12	2.21	0.41
2:I:521:LEU:HD22	2:I:667:LEU:HD12	2.02	0.41
2:I:976:ARG:HG3	2:I:989:LEU:HD23	2.03	0.41
4:K:13:ILE:HG21	4:K:19:LEU:HB2	2.02	0.41
5:L:324:LYS:HB3	5:L:325:PRO:HD2	2.03	0.41
5:L:402:LEU:HD12	5:L:402:LEU:HA	1.76	0.41
1:B:195:ARG:C	1:B:197:ASP:H	2.25	0.41
2:C:590:PRO:HD3	2:C:605:TYR:CE2	2.56	0.41
2:I:176:ILE:HD11	2:I:428:VAL:HG21	2.03	0.41
3:J:118:LYS:HB3	3:J:311:ARG:HD2	2.03	0.41
3:J:127:LEU:HD12	3:J:237:MET:HE1	2.03	0.41
2:C:342:ASP:HA	2:C:437:ASN:HB3	2.03	0.41
2:C:468:LEU:HD12	2:C:468:LEU:HA	1.94	0.41
2:C:939:VAL:O	2:C:941:LYS:N	2.53	0.41
3:D:513:MET:O	3:D:575:GLY:HA3	2.20	0.41
3:D:573:THR:O	3:D:577:ALA:N	2.43	0.41
3:D:842:ARG:NH2	3:D:1254:GLU:OE1	2.54	0.41
5:F:344:LEU:HD12	5:F:344:LEU:HA	1.82	0.41
1:H:37:HIS:HB3	2:I:1216:ARG:HB3	2.02	0.41
2:I:524:ILE:O	2:I:528:ARG:HG3	2.21	0.41
2:I:726:TYR:HB2	2:I:733:VAL:HB	2.02	0.41
2:I:754:THR:N	2:I:767:GLN:OE1	2.45	0.41
2:I:848:GLU:OE2	2:I:888:THR:OG1	2.39	0.41
3:J:267:ASP:O	3:J:271:ARG:HG3	2.21	0.41
3:J:312:ARG:HD3	3:J:312:ARG:HA	1.77	0.41
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:612:LEU:HD12	3:J:612:LEU:HA	1.96	0.41
4:K:36:ASP:O	4:K:38:LEU:N	2.54	0.41
4:K:40:PRO:C	4:K:42:GLU:H	2.29	0.41
5:L:311:THR:HG21	5:L:348:GLU:CD	2.46	0.41
2:C:548:ARG:NE	2:C:569:ILE:O	2.51	0.41
3:D:1146:GLU:CD	3:D:1310:THR:HG1	2.29	0.41
2:I:678:ARG:HD2	2:I:678:ARG:HA	1.86	0.41
2:I:870:ILE:HG21	2:I:944:ARG:CZ	2.51	0.41
2:C:27:LEU:HD23	2:C:27:LEU:HA	1.86	0.40
2:C:623:LEU:HD12	2:C:629:PHE:HA	2.03	0.40
2:C:1020:GLU:O	2:C:1024:GLU:HG2	2.21	0.40
3:D:233:LYS:HA	3:D:234:PRO:HD3	1.89	0.40
5:F:590:ILE:HG22	5:F:593:LYS:HE2	2.03	0.40
2:I:404:LYS:HE2	2:I:586:PHE:CZ	2.55	0.40
2:I:666:SER:HA	2:I:1186:VAL:HG21	2.03	0.40
2:I:1290:MET:HE1	3:J:469:HIS:CG	2.56	0.40
3:J:884:SER:OG	3:J:1254:GLU:OE1	2.34	0.40
2:C:559:CYS:HB2	2:C:662:SER:HB3	2.03	0.40
3:D:452:LEU:HG	3:D:625:MET:CE	2.48	0.40
3:D:514:THR:O	3:D:595:ALA:HA	2.21	0.40
3:D:686:TRP:CE3	3:D:758:PRO:HG3	2.56	0.40
3:D:899:TYR:O	3:D:1251:LYS:HD3	2.21	0.40
1:H:102:LEU:O	1:H:141:SER:HA	2.21	0.40
3:J:1225:GLY:O	3:J:1229:VAL:HG23	2.20	0.40
1:B:125:LYS:HA	1:B:126:PRO:HD2	1.94	0.40
2:C:1199:LEU:O	2:C:1203:ASP:N	2.54	0.40
2:C:1328:LYS:HA	2:C:1328:LYS:HD3	1.86	0.40
5:F:251:LYS:O	5:F:255:VAL:HG23	2.20	0.40
1:G:22:THR:HB	1:G:207:THR:O	2.21	0.40
1:H:47:LEU:HA	1:H:51:MET:HG2	2.03	0.40
2:I:1030:GLU:O	2:I:1034:ARG:HG3	2.21	0.40
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.83	0.40
1:A:32:GLU:HB2	1:A:35:PHE:CD2	2.56	0.40
2:C:151:ARG:HE	2:C:151:ARG:HB3	1.81	0.40
2:C:233:ARG:O	2:C:236:LYS:HG2	2.22	0.40
2:C:905:ILE:HD11	5:F:598:LEU:HD13	2.04	0.40
2:C:920:VAL:HA	2:C:921:PRO:HD3	1.90	0.40
3:D:114:ILE:HD11	3:D:311:ARG:HB3	2.02	0.40
3:J:232:ASN:ND2	3:J:1337:VAL:O	2.55	0.40
3:J:242:LEU:HA	3:J:243:PRO:HD3	1.92	0.40
5:L:415:ALA:HB2	5:L:434:TRP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:509:THR:HA	5:L:510:PRO:HD3	1.90	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	292/335 (87%)	268 (92%)	14 (5%)	10 (3%)	3	24
1	B	281/335 (84%)	257 (92%)	12 (4%)	12 (4%)	2	20
1	G	212/335 (63%)	193 (91%)	14 (7%)	5 (2%)	4	30
1	H	211/335 (63%)	195 (92%)	12 (6%)	4 (2%)	6	34
2	C	1338/1342 (100%)	1259 (94%)	60 (4%)	19 (1%)	9	39
2	I	1338/1342 (100%)	1257 (94%)	65 (5%)	16 (1%)	10	42
3	D	1141/1407 (81%)	1030 (90%)	75 (7%)	36 (3%)	3	25
3	J	1134/1407 (81%)	1026 (90%)	71 (6%)	37 (3%)	3	24
4	E	87/91 (96%)	72 (83%)	6 (7%)	9 (10%)	0	7
4	K	73/91 (80%)	61 (84%)	5 (7%)	7 (10%)	0	9
5	F	456/613 (74%)	437 (96%)	14 (3%)	5 (1%)	11	44
5	L	456/613 (74%)	436 (96%)	14 (3%)	6 (1%)	9	41
All	All	7019/8246 (85%)	6491 (92%)	362 (5%)	166 (2%)	4	30

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	188	GLU
1	A	229	GLU

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Mol	Chain	Res	Type
1	A	319	GLU
1	A	320	ASN
1	B	93	GLN
1	B	188	GLU
1	B	192	VAL
1	B	195	ARG
1	B	319	GLU
1	B	320	ASN
2	C	110	PRO
2	C	214	ASN
2	C	346	TYR
2	C	748	ILE
2	C	1040	ASP
3	D	151	MET
3	D	407	VAL
3	D	539	SER
3	D	588	PRO
3	D	833	GLU
3	D	851	PRO
3	D	859	PRO
3	D	880	VAL
3	D	1153	PRO
3	D	1168	GLU
3	D	1169	THR
3	D	1185	PRO
3	D	1190	ILE
3	D	1191	PRO
3	D	1214	PRO
4	E	16	ARG
4	E	36	ASP
4	E	37	PRO
4	E	40	PRO
4	E	80	LEU
5	F	488	LEU
5	F	490	PRO
1	G	93	GLN
1	G	188	GLU
1	G	231	PHE
1	H	93	GLN
1	H	188	GLU
2	I	9	LYS
2	I	110	PRO

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Mol	Chain	Res	Type
2	I	214	ASN
2	I	346	TYR
2	I	748	ILE
3	J	151	MET
3	J	407	VAL
3	J	528	THR
3	J	539	SER
3	J	587	LEU
3	J	588	PRO
3	J	833	GLU
3	J	851	PRO
3	J	859	PRO
3	J	880	VAL
3	J	1153	PRO
3	J	1168	GLU
3	J	1185	PRO
3	J	1190	ILE
3	J	1191	PRO
3	J	1214	PRO
4	K	36	ASP
4	K	37	PRO
4	K	40	PRO
5	L	488	LEU
5	L	490	PRO
1	A	191	ARG
1	A	323	PRO
1	B	7	GLU
1	B	191	ARG
2	C	909	LYS
2	C	940	GLU
2	C	1154	ASP
2	C	1155	VAL
3	D	555	TYR
3	D	825	VAL
3	D	906	GLY
3	D	1155	ILE
2	I	114	VAL
3	J	420	PRO
3	J	557	LYS
3	J	596	LEU
3	J	906	GLY
3	J	1149	ARG

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Mol	Chain	Res	Type
3	J	1160	SER
3	J	1161	GLY
3	J	1169	THR
3	J	1176	VAL
3	J	1209	VAL
1	A	192	VAL
1	B	13	LEU
1	B	157	THR
2	C	114	VAL
2	C	746	ALA
3	D	420	PRO
3	D	462	ASP
3	D	1150	PRO
4	E	45	LYS
4	E	60	ASN
4	E	79	GLU
5	F	307	THR
2	I	169	LYS
2	I	746	ALA
2	I	941	LYS
3	J	522	GLY
3	J	560	ASN
3	J	1215	GLU
4	K	45	LYS
4	K	60	ASN
5	L	307	THR
1	A	30	PRO
1	B	30	PRO
2	C	40	GLU
2	C	892	GLU
3	D	179	LYS
3	D	564	VAL
3	D	595	ALA
3	D	858	VAL
3	D	1160	SER
3	D	1176	VAL
3	D	1177	ILE
3	D	1208	ASP
2	I	40	GLU
2	I	891	GLY
3	J	462	ASP
3	J	1150	PRO

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Mol	Chain	Res	Type
4	K	15	ASN
4	K	59	ILE
5	L	212	ILE
1	A	230	ALA
1	B	193	GLU
2	C	49	LEU
2	C	61	SER
2	C	741	MET
2	C	1204	LEU
3	D	148	GLU
3	D	834	PRO
3	D	1149	ARG
1	G	29	GLU
1	H	29	GLU
2	I	1203	ASP
2	I	1204	LEU
3	J	593	ASN
3	J	718	SER
2	C	9	LYS
3	D	718	SER
1	H	30	PRO
2	I	741	MET
3	J	1177	ILE
2	C	1181	PRO
3	D	582	ILE
5	F	606	VAL
1	G	30	PRO
3	J	564	VAL
3	J	582	ILE
3	D	828	GLY
5	F	500	ILE
4	E	59	ILE
2	I	1155	VAL
2	I	1181	PRO
3	J	834	PRO
5	L	500	ILE
5	L	606	VAL

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	239/292 (82%)	221 (92%)	18 (8%)	12	37
1	B	233/292 (80%)	215 (92%)	18 (8%)	12	36
1	G	173/292 (59%)	163 (94%)	10 (6%)	18	44
1	H	171/292 (59%)	159 (93%)	12 (7%)	14	40
2	C	822/1157 (71%)	757 (92%)	65 (8%)	11	36
2	I	828/1157 (72%)	766 (92%)	62 (8%)	12	37
3	D	517/1168 (44%)	447 (86%)	70 (14%)	4	18
3	J	515/1168 (44%)	443 (86%)	72 (14%)	3	17
4	E	10/75 (13%)	8 (80%)	2 (20%)	1	9
4	K	9/75 (12%)	8 (89%)	1 (11%)	6	23
5	F	348/540 (64%)	309 (89%)	39 (11%)	6	23
5	L	348/540 (64%)	316 (91%)	32 (9%)	8	30
All	All	4213/7048 (60%)	3812 (90%)	401 (10%)	8	29

All (401) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	14	VAL
1	A	29	GLU
1	A	67	GLU
1	A	88	LEU
1	A	95	LYS
1	A	102	LEU
1	A	117	HIS
1	A	131	CYS
1	A	140	ILE
1	A	171	LEU
1	A	173	VAL
1	A	178	SER
1	A	210	THR
1	A	287	VAL
1	A	318	LEU
1	A	319	GLU
1	A	321	TRP

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Mol	Chain	Res	Type
1	B	12	ARG
1	B	29	GLU
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	196	THR
1	B	205	MET
1	B	210	THR
1	B	287	VAL
1	B	318	LEU
1	B	319	GLU
1	B	321	TRP
2	C	15	PHE
2	C	24	VAL
2	C	71	VAL
2	C	79	VAL
2	C	82	VAL
2	C	90	VAL
2	C	117	ILE
2	C	135	THR
2	C	144	VAL
2	C	151	ARG
2	C	374	GLU
2	C	378	ARG
2	C	451	ARG
2	C	456	VAL
2	C	478	ARG
2	C	486	THR
2	C	525	THR
2	C	529	ARG
2	C	530	ILE
2	C	538	LEU
2	C	539	THR
2	C	541	GLU
2	C	542	ARG
2	C	547	VAL

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Mol	Chain	Res	Type
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	623	LEU
2	C	634	VAL
2	C	635	THR
2	C	657	THR
2	C	666	SER
2	C	692	THR
2	C	694	ARG
2	C	705	GLU
2	C	717	VAL
2	C	723	VAL
2	C	754	THR
2	C	761	GLN
2	C	776	PRO
2	C	818	VAL
2	C	823	VAL
2	C	830	THR
2	C	878	THR
2	C	896	THR
2	C	902	LEU
2	C	917	SER
2	C	936	ARG
2	C	1029	LEU
2	C	1042	LEU
2	C	1056	VAL
2	C	1075	VAL
2	C	1186	VAL
2	C	1191	LYS
2	C	1197	GLU
2	C	1216	ARG
2	C	1226	THR
2	C	1239	VAL
2	C	1250	SER
2	C	1293	VAL
2	C	1298	VAL
2	C	1302	THR
3	D	42	GLU

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Mol	Chain	Res	Type
3	D	58	CYS
3	D	83	VAL
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	208	THR
3	D	218	THR
3	D	232	ASN
3	D	240	THR
3	D	250	ARG
3	D	254	PRO
3	D	272	VAL
3	D	301	GLU
3	D	311	ARG
3	D	312	ARG
3	D	352	ARG
3	D	392	THR
3	D	401	VAL
3	D	419	HIS
3	D	420	PRO
3	D	430	HIS
3	D	491	LEU
3	D	514	THR
3	D	607	THR
3	D	612	LEU
3	D	616	PRO
3	D	635	SER
3	D	646	ILE
3	D	648	GLU
3	D	661	VAL
3	D	673	VAL
3	D	674	THR
3	D	690	ASN
3	D	721	SER
3	D	738	ARG
3	D	739	GLN
3	D	743	MET
3	D	753	SER
3	D	764	ARG

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Mol	Chain	Res	Type
3	D	767	LEU
3	D	769	VAL
3	D	777	HIS
3	D	781	LYS
3	D	783	LEU
3	D	785	ASP
3	D	786	THR
3	D	790	THR
3	D	808	VAL
3	D	810	THR
3	D	816	THR
3	D	842	ARG
3	D	844	THR
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	886	VAL
3	D	890	THR
3	D	894	VAL
3	D	913	GLU
3	D	1226	VAL
3	D	1247	LYS
3	D	1265	THR
3	D	1316	THR
4	E	4	VAL
4	E	10	VAL
5	F	107	THR
5	F	154	GLU
5	F	158	LEU
5	F	159	SER
5	F	162	ILE
5	F	213	ASP
5	F	218	ARG
5	F	235	ILE
5	F	242	HIS
5	F	250	LEU
5	F	262	VAL
5	F	264	LYS
5	F	273	MET

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Mol	Chain	Res	Type
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	397	ARG
5	F	420	GLU
5	F	425	TYR
5	F	426	LYS
5	F	437	GLN
5	F	479	THR
5	F	480	PRO
5	F	513	ASP
5	F	526	THR
5	F	527	THR
5	F	537	THR
5	F	544	THR
5	F	551	LEU
5	F	552	THR
5	F	554	ARG
5	F	559	LEU
5	F	569	THR
5	F	584	ARG
5	F	589	GLN
5	F	597	LYS
1	G	14	VAL
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	182	ARG
1	H	14	VAL
1	H	88	LEU
1	H	95	LYS
1	H	102	LEU
1	H	117	HIS
1	H	131	CYS

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Mol	Chain	Res	Type
1	H	140	ILE
1	H	171	LEU
1	H	173	VAL
1	H	182	ARG
1	H	210	THR
1	H	211	ILE
2	I	15	PHE
2	I	24	VAL
2	I	79	VAL
2	I	144	VAL
2	I	151	ARG
2	I	374	GLU
2	I	378	ARG
2	I	451	ARG
2	I	456	VAL
2	I	478	ARG
2	I	529	ARG
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	541	GLU
2	I	547	VAL
2	I	574	SER
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	657	THR
2	I	666	SER
2	I	692	THR
2	I	694	ARG
2	I	705	GLU
2	I	717	VAL
2	I	723	VAL
2	I	761	GLN
2	I	776	PRO
2	I	782	VAL
2	I	789	THR
2	I	818	VAL
2	I	822	VAL

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Mol	Chain	Res	Type
2	I	823	VAL
2	I	839	VAL
2	I	857	VAL
2	I	888	THR
2	I	893	THR
2	I	896	THR
2	I	902	LEU
2	I	903	ARG
2	I	917	SER
2	I	936	ARG
2	I	1029	LEU
2	I	1042	LEU
2	I	1056	VAL
2	I	1075	VAL
2	I	1184	THR
2	I	1186	VAL
2	I	1191	LYS
2	I	1197	GLU
2	I	1216	ARG
2	I	1226	THR
2	I	1239	VAL
2	I	1250	SER
2	I	1262	LYS
2	I	1293	VAL
2	I	1298	VAL
2	I	1302	THR
3	J	42	GLU
3	J	58	CYS
3	J	83	VAL
3	J	92	VAL
3	J	93	THR
3	J	114	ILE
3	J	118	LYS
3	J	167	ASP
3	J	191	SER
3	J	193	ASP
3	J	232	ASN
3	J	250	ARG
3	J	254	PRO
3	J	301	GLU
3	J	311	ARG
3	J	312	ARG

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Mol	Chain	Res	Type
3	J	319	SER
3	J	352	ARG
3	J	374	LEU
3	J	393	THR
3	J	419	HIS
3	J	430	HIS
3	J	491	LEU
3	J	501	VAL
3	J	514	THR
3	J	607	THR
3	J	612	LEU
3	J	616	PRO
3	J	635	SER
3	J	646	ILE
3	J	648	GLU
3	J	661	VAL
3	J	673	VAL
3	J	674	THR
3	J	690	ASN
3	J	721	SER
3	J	738	ARG
3	J	739	GLN
3	J	740	LEU
3	J	743	MET
3	J	753	SER
3	J	760	THR
3	J	764	ARG
3	J	767	LEU
3	J	769	VAL
3	J	776	THR
3	J	777	HIS
3	J	781	LYS
3	J	783	LEU
3	J	785	ASP
3	J	786	THR
3	J	790	THR
3	J	808	VAL
3	J	810	THR
3	J	816	THR
3	J	842	ARG
3	J	862	THR
3	J	864	LEU

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Mol	Chain	Res	Type
3	J	869	CYS
3	J	877	VAL
3	J	880	VAL
3	J	882	VAL
3	J	885	VAL
3	J	894	VAL
3	J	903	LEU
3	J	913	GLU
3	J	1226	VAL
3	J	1247	LYS
3	J	1265	THR
3	J	1280	VAL
3	J	1316	THR
3	J	1353	VAL
4	K	4	VAL
5	L	107	THR
5	L	154	GLU
5	L	158	LEU
5	L	159	SER
5	L	162	ILE
5	L	218	ARG
5	L	242	HIS
5	L	250	LEU
5	L	264	LYS
5	L	273	MET
5	L	311	THR
5	L	333	VAL
5	L	336	GLU
5	L	354	THR
5	L	360	ASP
5	L	397	ARG
5	L	420	GLU
5	L	425	TYR
5	L	437	GLN
5	L	446	GLN
5	L	479	THR
5	L	480	PRO
5	L	497	VAL
5	L	513	ASP
5	L	544	THR
5	L	552	THR
5	L	554	ARG

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Mol	Chain	Res	Type
5	L	559	LEU
5	L	569	THR
5	L	584	ARG
5	L	589	GLN
5	L	597	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	75	GLN
1	A	128	HIS
1	A	227	GLN
1	A	283	GLN
1	A	294	ASN
1	A	320	ASN
1	B	37	HIS
1	B	41	ASN
1	B	66	HIS
1	B	128	HIS
1	B	227	GLN
1	B	276	HIS
1	B	283	GLN
1	B	320	ASN
2	C	139	ASN
2	C	150	HIS
2	C	235	ASN
2	C	437	ASN
2	C	554	HIS
2	C	618	GLN
2	C	659	GLN
2	C	677	ASN
2	C	832	HIS
2	C	955	GLN
2	C	1013	GLN
2	C	1023	HIS
2	C	1061	GLN
2	C	1257	GLN
3	D	113	HIS
3	D	294	ASN
3	D	477	GLN
3	D	690	ASN

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Mol	Chain	Res	Type
3	D	777	HIS
3	D	865	HIS
3	D	1218	HIS
3	D	1326	GLN
5	F	128	ASN
5	F	129	GLN
5	F	131	GLN
5	F	227	GLN
5	F	283	GLN
5	F	309	ASN
5	F	357	GLN
5	F	383	ASN
5	F	437	GLN
5	F	455	HIS
5	F	472	GLN
1	G	75	GLN
1	G	128	HIS
1	H	37	HIS
1	H	41	ASN
1	H	66	HIS
1	H	75	GLN
1	H	128	HIS
2	I	139	ASN
2	I	150	HIS
2	I	235	ASN
2	I	437	ASN
2	I	554	HIS
2	I	677	ASN
2	I	955	GLN
2	I	1013	GLN
2	I	1017	GLN
2	I	1023	HIS
2	I	1061	GLN
3	J	435	GLN
3	J	477	GLN
3	J	690	ASN
3	J	739	GLN
3	J	777	HIS
3	J	897	HIS
3	J	929	GLN
3	J	1326	GLN
5	L	128	ASN

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Mol	Chain	Res	Type
5	L	129	GLN
5	L	131	GLN
5	L	227	GLN
5	L	283	GLN
5	L	309	ASN
5	L	331	HIS
5	L	357	GLN
5	L	383	ASN
5	L	437	GLN
5	L	589	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 oligosaccharides 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 [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	298/335 (88%)	-0.11	2 (0%) 84 68	27, 114, 296, 459	0
1	B	287/335 (85%)	0.18	15 (5%) 33 26	36, 191, 420, 550	0
1	G	216/335 (64%)	0.02	3 (1%) 73 53	33, 168, 289, 370	0
1	H	215/335 (64%)	0.20	8 (3%) 45 32	68, 188, 341, 524	0
2	C	1340/1342 (99%)	-0.02	30 (2%) 62 44	2, 102, 402, 550	1 (0%)
2	I	1340/1342 (99%)	0.03	36 (2%) 56 39	3, 144, 388, 550	1 (0%)
3	D	1147/1407 (81%)	-0.16	18 (1%) 70 50	3, 72, 236, 550	0
3	J	1140/1407 (81%)	-0.08	22 (1%) 66 47	3, 96, 268, 550	0
4	E	89/91 (97%)	-0.19	1 (1%) 78 58	6, 76, 206, 285	0
4	K	75/91 (82%)	0.08	3 (4%) 42 31	47, 171, 393, 535	0
5	F	464/613 (75%)	-0.04	5 (1%) 78 58	21, 149, 369, 550	0
5	L	464/613 (75%)	-0.09	4 (0%) 81 62	31, 169, 397, 550	0
All	All	7075/8246 (85%)	-0.04	147 (2%) 63 45	2, 121, 352, 550	2 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	9	LYS	5.5
1	B	309	SER	5.4
2	C	944	ARG	5.0
2	I	596	ASP	4.6
2	I	1312	ASN	4.5
2	C	56	VAL	4.4
2	I	944	ARG	4.2
3	J	575	GLY	4.2
5	F	597	LYS	4.2
2	C	292	ILE	4.2
2	I	1325	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	C	856	ASN	3.9
3	J	825	VAL	3.8
3	D	1294	ALA	3.8
2	C	65	ASN	3.7
2	I	1060	ILE	3.6
2	I	787	PRO	3.6
2	I	1072	ASN	3.5
3	J	249	LEU	3.5
1	H	146	VAL	3.5
3	J	218	THR	3.5
3	D	481	ARG	3.5
2	I	1183	ALA	3.4
3	D	139	LEU	3.4
3	J	631	TYR	3.3
3	J	512	TYR	3.3
1	H	205	MET	3.3
5	F	612	ASP	3.3
2	I	334	GLU	3.3
2	C	205	PRO	3.2
5	F	460	ILE	3.2
1	B	201	LEU	3.1
3	D	69	GLU	3.1
3	D	90	VAL	3.0
1	B	6	THR	3.0
2	C	52	ALA	3.0
3	D	68	TYR	3.0
3	J	1208	ASP	3.0
2	I	333	ILE	2.9
3	J	529	GLY	2.9
2	I	450	ASN	2.9
1	H	61	ILE	2.9
1	A	29	GLU	2.9
1	B	305	ASP	2.9
2	C	488	MET	2.8
2	I	389	PHE	2.8
2	I	388	LEU	2.8
3	J	481	ARG	2.8
1	G	83	LEU	2.8
2	I	562	GLU	2.8
4	K	16	ARG	2.7
2	I	1314	GLN	2.7
2	I	442	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	1021	LEU	2.7
2	I	664	GLY	2.7
1	H	217	ILE	2.7
2	I	1095	ASP	2.7
2	C	287	VAL	2.6
1	B	146	VAL	2.6
3	D	155	GLU	2.6
2	I	9	LYS	2.6
1	H	26	VAL	2.6
2	I	488	MET	2.6
3	D	520	ALA	2.6
2	I	449	GLY	2.6
1	B	203	ILE	2.6
3	J	526	VAL	2.5
3	D	822	MET	2.5
2	I	1190	ALA	2.5
3	J	1244	GLN	2.5
3	J	626	TYR	2.5
1	B	26	VAL	2.5
2	C	967	LEU	2.5
2	C	350	THR	2.5
3	J	395	LYS	2.4
1	B	217	ILE	2.4
3	J	182	ALA	2.4
3	D	719	PHE	2.4
5	F	228	TYR	2.4
2	I	915	ASP	2.4
5	F	381	GLU	2.4
3	J	482	ALA	2.4
3	D	593	ASN	2.4
5	L	527	THR	2.4
2	I	1122	LYS	2.4
2	I	771	VAL	2.3
2	C	42	ASP	2.3
2	I	1313	HIS	2.3
5	L	416	VAL	2.3
3	D	1230	THR	2.3
1	A	86	LYS	2.3
3	J	220	ARG	2.3
1	H	90	VAL	2.3
1	B	63	GLY	2.3
2	C	12	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	1067	ALA	2.3
1	B	67	GLU	2.3
1	H	37	HIS	2.2
2	C	209	ILE	2.2
2	I	142	GLU	2.2
3	J	516	ASP	2.2
2	I	605	TYR	2.2
2	C	288	PRO	2.2
3	D	482	ALA	2.2
1	B	261	GLU	2.2
2	C	354	ASP	2.2
3	J	593	ASN	2.2
2	C	875	ALA	2.2
2	I	837	ALA	2.2
5	L	315	TRP	2.2
4	E	32	VAL	2.2
2	I	998	LEU	2.2
2	I	15	PHE	2.2
3	J	863	LEU	2.2
1	G	68	TYR	2.1
2	I	877	VAL	2.1
3	D	825	VAL	2.1
3	D	324	LEU	2.1
2	C	686	GLN	2.1
2	C	1313	HIS	2.1
2	C	877	VAL	2.1
2	C	1018	TYR	2.1
2	I	555	TYR	2.1
2	C	336	LEU	2.1
1	G	144	ILE	2.1
2	C	230	PHE	2.1
2	C	153	PRO	2.1
2	I	827	ARG	2.1
5	L	447	ALA	2.1
3	J	509	GLY	2.1
2	C	558	VAL	2.1
2	C	291	TYR	2.1
2	C	942	ASP	2.1
1	H	193	GLU	2.1
4	K	7	GLN	2.1
2	C	960	LEU	2.1
1	B	209	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
4	K	40	PRO	2.0
1	B	259	ASP	2.0
2	I	641	GLU	2.0
3	D	846	GLU	2.0
3	J	685	ILE	2.0
1	B	224	LEU	2.0
3	D	220	ARG	2.0
3	D	176	PHE	2.0
3	J	770	LEU	2.0
1	B	202	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	J	2000	1/1	-0.30	0.29	396,396,396,396	0
6	MG	D	2000	1/1	0.18	0.20	320,320,320,320	0
7	ZN	D	2001	1/1	1.00	0.02	83,83,83,83	0
7	ZN	D	2002	1/1	1.00	0.02	68,68,68,68	0
7	ZN	J	2001	1/1	1.00	0.01	104,104,104,104	0
7	ZN	J	2002	1/1	1.00	0.03	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.