



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:04 PM GMT

PDB ID : 4BBR
Title : Structure of RNA polymerase II-TFIIB complex
Authors : Sainsbury, S.; Niesser, J.; Cramer, P.
Deposited on : 2012-09-27
Resolution : 3.40 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 ⓘ](#)) 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

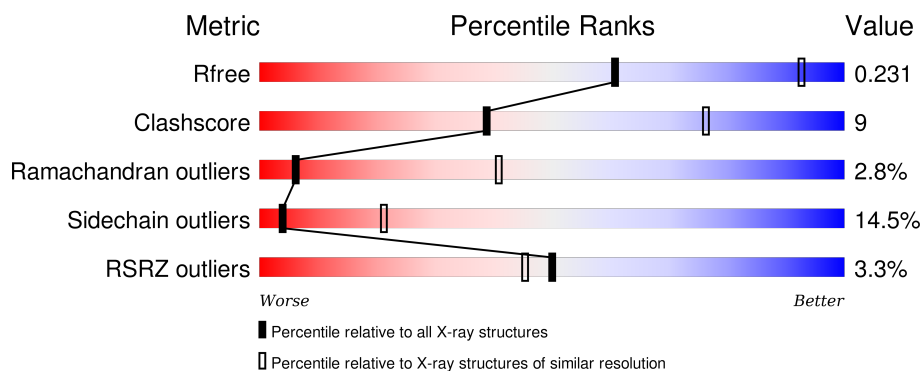
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1733	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>21%</div> <div>• •</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>26%</div> <div>•</div> <div>6%</div> </div> </div>
3	C	318	<div> <div>•</div> <div> <div></div> <div>59%</div> <div>22%</div> <div>•</div> <div>16%</div> </div> </div>
4	D	221	<div> <div>•</div> <div> <div></div> <div>55%</div> <div>19%</div> <div>6%</div> <div>19%</div> </div> </div>
5	E	215	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>22%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	

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
15	MG	A	2458	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 32800 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 II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1414	Total	C	N	O	S	0	0	0
			11123	7007	1945	2109	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	0	0	0
			9095	5751	1598	1690	56			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	193	Total	C	N	O	S	0	0	0
			1396	862	246	274	14			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	Zn	0	0
			1	1		
14	B	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	C	1	Total	Zn	0	0
			1	1		
14	A	2	Total	Zn	0	0
			2	2		
14	L	1	Total	Zn	0	0
			1	1		
14	M	1	Total	Zn	0	0
			1	1		

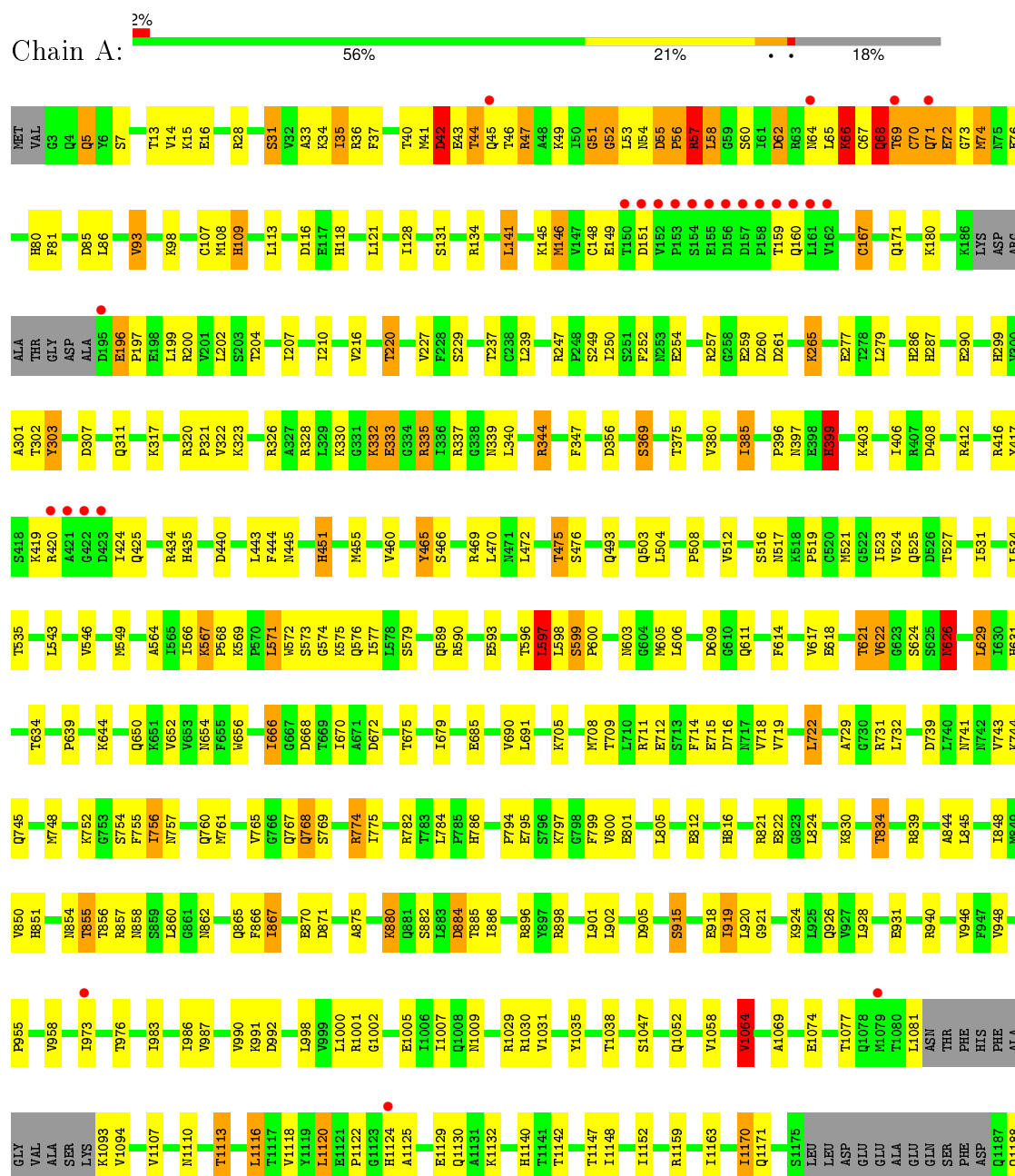
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

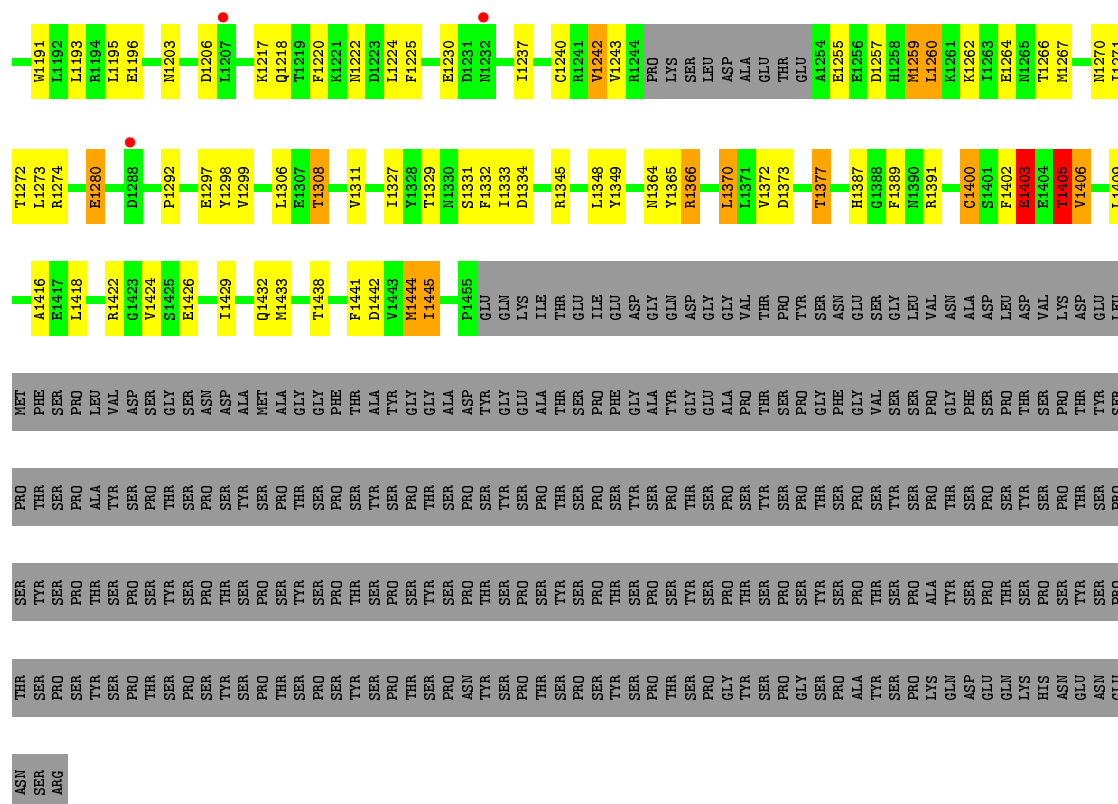
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

3 Residue-property plots

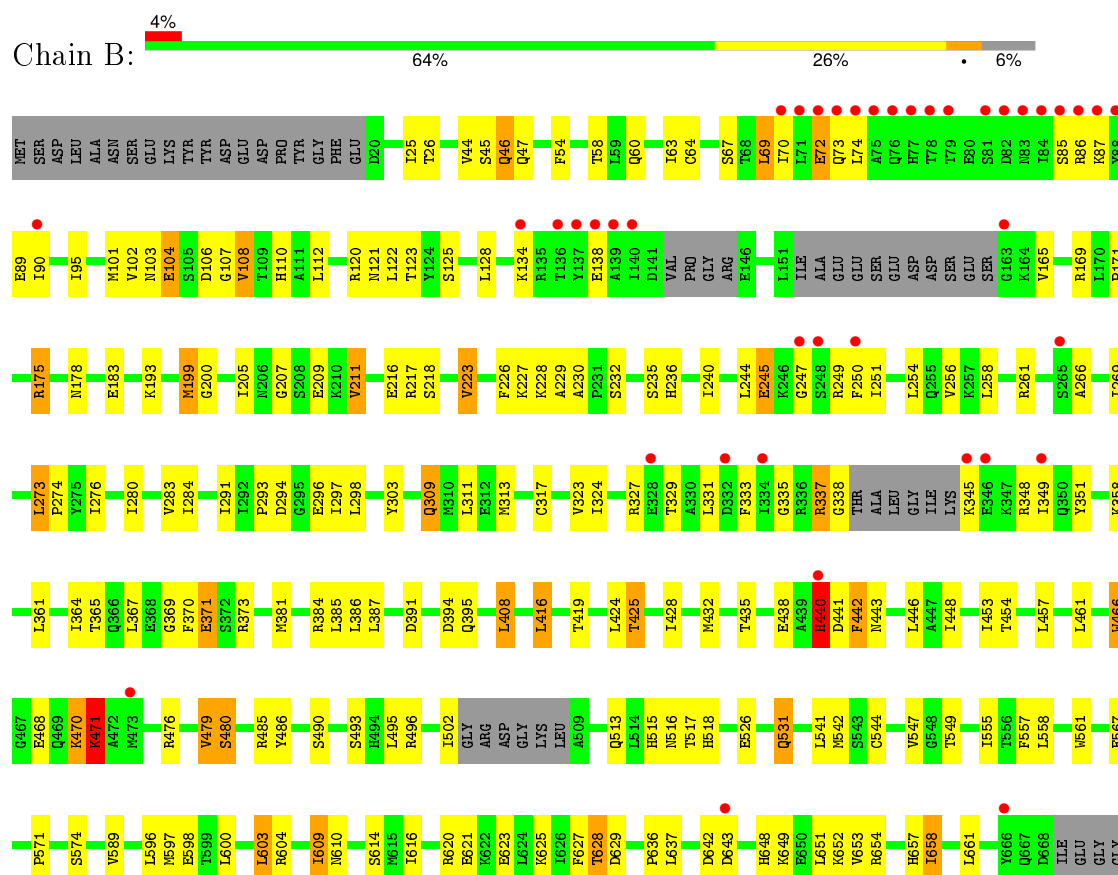
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

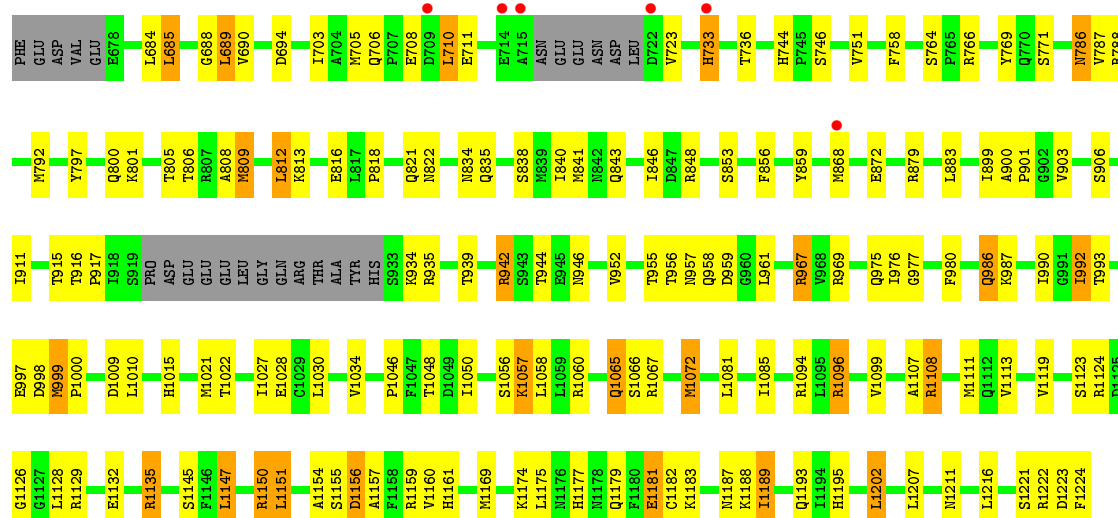
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



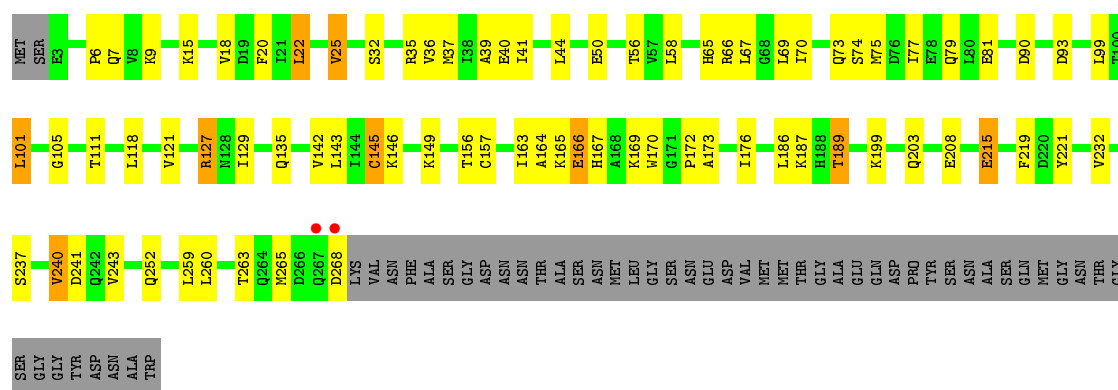


• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

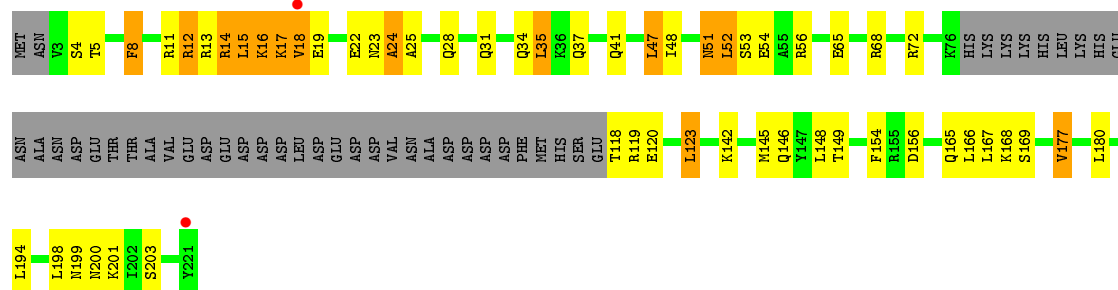




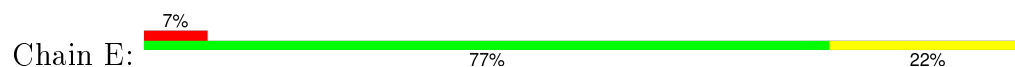
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

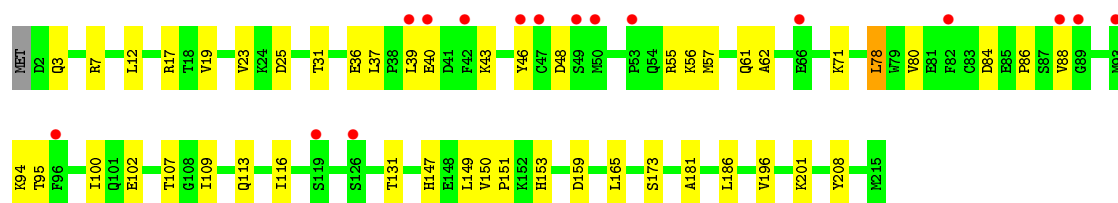


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

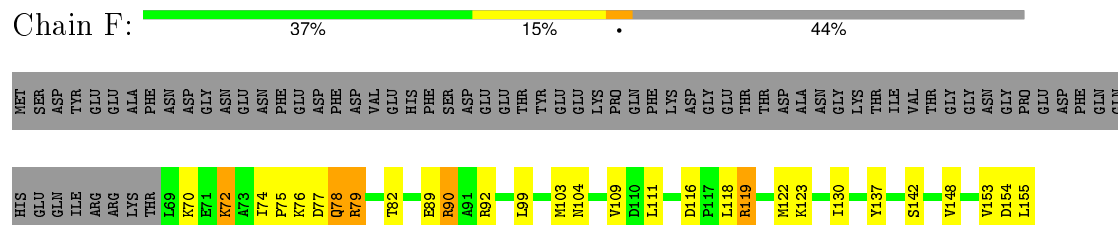


• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

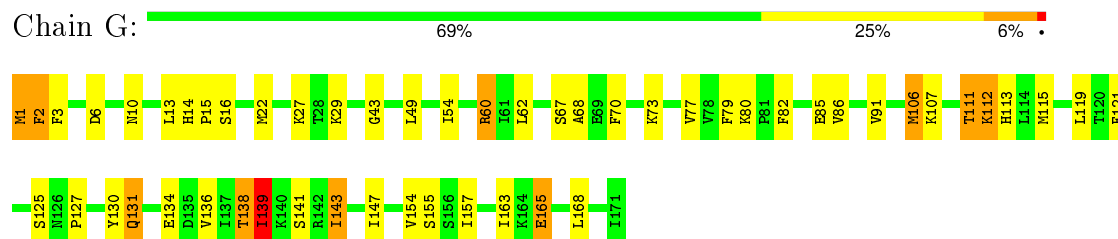




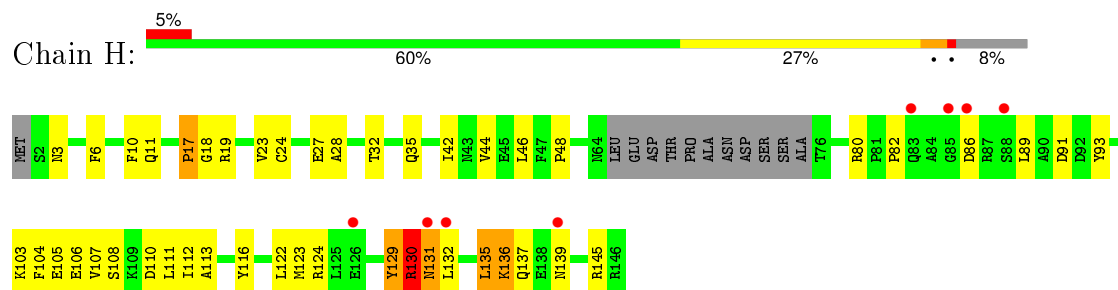
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



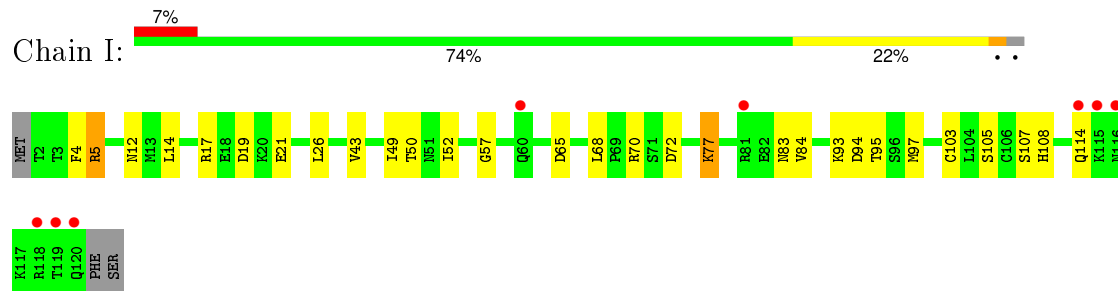
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



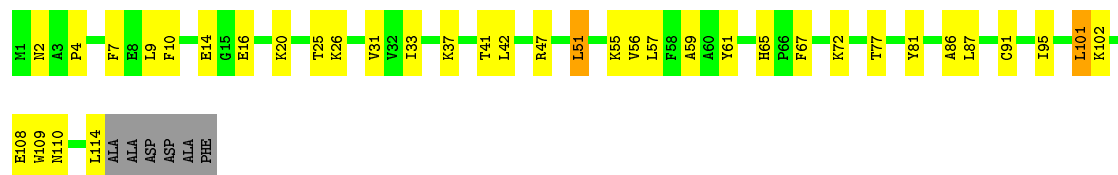
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5





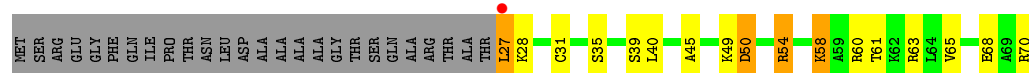
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K: 64% 29% 5%



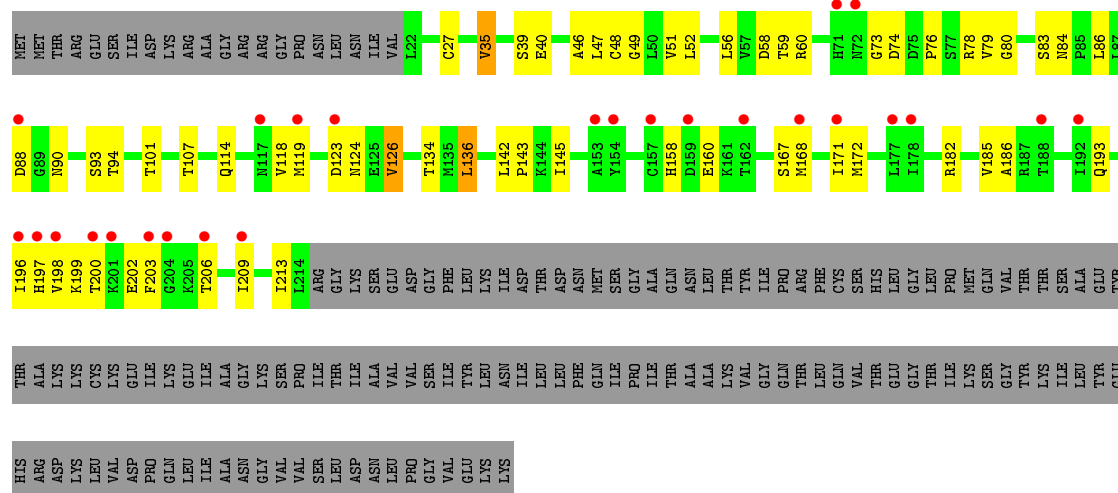
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 39% 19% 6% 37%



• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

Chain M: 8% 39% 17% 44%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.44Å 386.76Å 254.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 3.40 49.41 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.41-3.40) 100.0 (49.41-3.40)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.174 , 0.211 0.193 , 0.231	Depositor DCC
R_{free} test set	2994 reflections (2.00%)	DCC
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 86.6	EDS
Estimated twinning fraction	0.025 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.029 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 149749 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32800	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	2/11322 (0.0%)	0.81	6/15312 (0.0%)
2	B	0.50	0/9271	0.80	2/12505 (0.0%)
3	C	0.53	0/2133	0.81	0/2891
4	D	0.55	0/1444	0.88	1/1935 (0.1%)
5	E	0.45	0/1788	0.71	0/2406
6	F	0.53	0/717	0.78	0/967
7	G	0.52	0/1368	0.82	0/1844
8	H	0.49	0/1094	0.81	0/1481
9	I	0.44	0/989	0.77	0/1331
10	J	0.61	0/541	0.91	0/727
11	K	0.50	0/937	0.70	0/1265
12	L	0.52	0/353	0.89	0/468
13	M	0.50	0/1413	0.85	0/1916
All	All	0.51	2/33370 (0.0%)	0.81	9/45048 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	6.57	1.95	1.50
1	A	57	ARG	CA-C	5.52	1.67	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	470	LYS	C-N-CA	6.89	138.91	121.70
1	A	56	PRO	C-N-CA	6.71	138.47	121.70
1	A	399	HIS	N-CA-CB	5.53	120.55	110.60
1	A	1403	GLU	N-CA-C	5.40	125.59	111.00
1	A	332	LYS	N-CA-C	-5.21	96.93	111.00
1	A	55	ASP	N-CA-CB	5.21	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	628	THR	C-N-CA	5.15	134.57	121.70
4	D	24	ALA	N-CA-C	5.09	124.75	111.00
1	A	57	ARG	CA-CB-CG	5.04	124.49	113.40

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	11123	0	11184	240	0
2	B	9095	0	9055	180	0
3	C	2095	0	2051	43	0
4	D	1434	0	1460	26	0
5	E	1752	0	1776	18	0
6	F	705	0	731	19	0
7	G	1340	0	1357	34	0
8	H	1076	0	1046	23	0
9	I	971	0	927	12	0
10	J	532	0	542	27	0
11	K	919	0	929	26	0
12	L	351	0	374	13	0
13	M	1396	0	1312	19	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
14	M	1	0	0	0	0
15	A	2	0	0	0	0
All	All	32800	0	32744	592	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 9.

All (592) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.95	1.41
2:B:515:HIS:HD2	2:B:517:THR:H	1.04	0.93
11:K:65:HIS:HD2	11:K:67:PHE:H	1.09	0.92
12:L:61:THR:HB	12:L:63:ARG:HG3	1.53	0.90
2:B:955:THR:HG22	2:B:956:THR:H	1.33	0.90
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.54	0.89
2:B:470:LYS:HB2	2:B:471:LYS:HB2	1.53	0.88
2:B:515:HIS:CD2	2:B:517:THR:H	1.93	0.85
1:A:57:ARG:O	1:A:68:GLN:HG2	1.77	0.84
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.44	0.83
1:A:855:THR:HG21	1:A:857:ARG:HE	1.43	0.83
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.60	0.82
7:G:1:MET:CE	7:G:80:LYS:H	1.93	0.81
7:G:138:THR:HG22	7:G:139:ILE:H	1.45	0.81
2:B:986:GLN:HE22	2:B:1022:THR:HG21	1.46	0.80
8:H:130:ARG:H	8:H:130:ARG:HD3	1.47	0.78
3:C:73:GLN:HE21	3:C:75:MET:H	1.32	0.78
1:A:406:ILE:HG12	1:A:412:ARG:HG3	1.65	0.78
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.65	0.77
6:F:155:LEU:H	6:F:155:LEU:HD12	1.51	0.76
1:A:1329:THR:HG22	1:A:1331:SER:H	1.50	0.75
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.67	0.75
1:A:56:PRO:O	1:A:57:ARG:HD2	1.87	0.74
4:D:145:MET:O	4:D:149:THR:HG22	1.86	0.74
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.69	0.74
2:B:303:TYR:HD1	2:B:571:PRO:HB3	1.52	0.74
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	1.87	0.74
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.69	0.74
1:A:880:LYS:HE3	1:A:955:PRO:HG3	1.68	0.74
11:K:65:HIS:CD2	11:K:67:PHE:H	2.00	0.72
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.69	0.72
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.72
1:A:216:VAL:O	1:A:220:THR:HB	1.90	0.72
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.71	0.71
2:B:955:THR:HG22	2:B:956:THR:N	2.06	0.71
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.73	0.70
8:H:129:TYR:H	8:H:129:TYR:HD1	1.37	0.70
2:B:486:TYR:HA	2:B:1096:ARG:HH22	1.56	0.70
2:B:438:GLU:HG3	2:B:440:HIS:HB2	1.72	0.70
7:G:1:MET:HE1	7:G:80:LYS:H	1.57	0.70
13:M:193:GLN:HA	13:M:198:VAL:HB	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:74:ILE:HD11	6:F:142:SER:HB3	1.74	0.70
7:G:1:MET:CE	7:G:2:PHE:H	2.04	0.69
7:G:1:MET:HE1	7:G:79:PHE:HA	1.73	0.69
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.75	0.69
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.73	0.68
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.74	0.68
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.74	0.68
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.75	0.68
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.76	0.68
13:M:203:PHE:HA	13:M:206:THR:HG22	1.76	0.68
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.75	0.68
2:B:516:ASN:HD22	2:B:516:ASN:H	1.42	0.67
1:A:741:ASN:HD22	1:A:744:LYS:H	1.42	0.67
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.59	0.67
1:A:1120:LEU:HD13	1:A:1125:ALA:HA	1.78	0.66
2:B:86:ARG:HG2	2:B:138:GLU:HG3	1.77	0.66
1:A:709:THR:HB	1:A:712:GLU:H	1.61	0.66
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.30	0.66
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.30	0.66
2:B:236:HIS:HD2	2:B:258:LEU:HD23	1.59	0.66
1:A:567:LYS:HG3	1:A:568:PRO:HA	1.76	0.66
2:B:235:SER:HA	2:B:261:ARG:HH21	1.60	0.66
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.77	0.65
2:B:744:HIS:HD2	2:B:746:SER:H	1.45	0.65
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.93	0.65
1:A:108:MET:H	1:A:171:GLN:HE22	1.44	0.65
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.79	0.65
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.78	0.65
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.79	0.65
8:H:6:PHE:HD1	8:H:130:ARG:HG2	1.61	0.64
2:B:900:ALA:HB3	12:L:61:THR:HG22	1.80	0.64
1:A:65:LEU:HD23	1:A:71:GLN:HB3	1.78	0.64
1:A:60:SER:HB2	1:A:67:CYS:HB2	1.80	0.64
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.79	0.63
1:A:1152:ILE:HG12	1:A:1260:LEU:HD23	1.80	0.63
4:D:52:LEU:HB3	4:D:148:LEU:HD23	1.81	0.63
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.81	0.63
2:B:515:HIS:H	2:B:518:HIS:CD2	2.16	0.63
2:B:955:THR:CG2	2:B:956:THR:H	2.10	0.63
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.80	0.63
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.82	0.62
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.81	0.62
2:B:64:CYS:HA	2:B:67:SER:HB3	1.80	0.62
7:G:115:MET:HG2	7:G:119:LEU:HD23	1.81	0.61
8:H:131:ASN:HD22	8:H:132:LEU:H	1.47	0.61
2:B:104:GLU:HG3	12:L:54:ARG:NH1	2.15	0.61
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.82	0.61
2:B:801:LYS:O	10:J:52:THR:HG23	2.00	0.61
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.63	0.61
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.83	0.61
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.33	0.61
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.82	0.61
2:B:705:MET:H	2:B:710:LEU:HG	1.66	0.60
12:L:28:LYS:HB2	12:L:39:SER:HA	1.83	0.60
7:G:1:MET:HE3	7:G:80:LYS:H	1.66	0.60
2:B:901:PRO:HD3	12:L:58:LYS:HB3	1.82	0.60
2:B:70:ILE:HG22	2:B:89:GLU:HG2	1.83	0.60
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.84	0.60
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.84	0.59
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.84	0.59
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.82	0.59
9:I:103:CYS:O	9:I:107:SER:HA	2.02	0.59
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.84	0.59
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.82	0.59
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.84	0.59
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.35	0.59
1:A:854:ASN:HB2	1:A:1000:LEU:HD21	1.85	0.59
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.85	0.59
6:F:72:LYS:HB2	6:F:142:SER:HA	1.84	0.58
1:A:229:SER:HB3	1:A:1416:ALA:HB2	1.85	0.58
7:G:1:MET:HE2	7:G:2:PHE:H	1.68	0.58
4:D:35:LEU:HA	4:D:47:LEU:HB2	1.85	0.58
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.86	0.58
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.69	0.58
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.85	0.58
2:B:1188:LYS:H	2:B:1189:ILE:HD12	1.69	0.58
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.85	0.58
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.86	0.57
1:A:549:MET:CE	1:A:656:TRP:HD1	2.17	0.57
6:F:77:ASP:O	6:F:78:GLN:HB2	2.04	0.57
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:915:THR:O	2:B:917:PRO:HD3	2.04	0.57
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.87	0.57
7:G:1:MET:SD	7:G:2:PHE:N	2.67	0.57
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.35	0.57
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.86	0.57
2:B:125:SER:HA	2:B:171:PRO:HA	1.86	0.57
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.35	0.57
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.86	0.57
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.70	0.57
2:B:324:ILE:HG13	2:B:329:THR:HG22	1.86	0.57
1:A:1329:THR:HG22	1:A:1331:SER:N	2.20	0.56
2:B:171:PRO:HG2	2:B:461:LEU:HD12	1.87	0.56
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.70	0.56
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.56
2:B:486:TYR:CA	2:B:1096:ARG:HH22	2.17	0.56
4:D:123:LEU:HD11	4:D:146:GLN:HG2	1.86	0.56
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.87	0.56
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.41	0.56
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.87	0.56
7:G:131:GLN:HG3	7:G:136:VAL:HG22	1.87	0.56
1:A:227:VAL:HG12	4:D:15:LEU:HD23	1.88	0.56
2:B:614:SER:HB3	2:B:627:PHE:HB2	1.87	0.56
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.06	0.56
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.89	0.56
3:C:32:SER:O	3:C:36:VAL:HG23	2.05	0.56
1:A:589:GLN:HG3	1:A:606:LEU:HD13	1.88	0.55
1:A:69:THR:HG22	2:B:1174:LYS:HD3	1.88	0.55
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.88	0.55
1:A:590:ARG:HH21	1:A:621:THR:HG23	1.72	0.55
1:A:672:ASP:OD1	1:A:675:THR:HB	2.06	0.55
2:B:797:TYR:O	10:J:1:MET:HG2	2.06	0.55
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.71	0.55
1:A:524:VAL:HG12	1:A:525:GLN:N	2.22	0.55
1:A:472:LEU:O	1:A:475:THR:HB	2.06	0.55
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.89	0.55
1:A:858:ASN:ND2	1:A:862:ASN:HB2	2.22	0.55
2:B:557:PHE:O	2:B:561:TRP:HD1	1.90	0.55
1:A:650:GLN:O	1:A:654:ASN:HB2	2.06	0.55
2:B:291:ILE:HG23	2:B:296:GLU:HB3	1.89	0.55
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.72	0.55
1:A:58:LEU:HD22	1:A:80:HIS:O	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:ASN:HD22	10:J:52:THR:HG21	1.71	0.55
5:E:19:VAL:O	5:E:23:VAL:HG23	2.06	0.55
1:A:866:PHE:HB3	1:A:867:ILE:HD12	1.89	0.54
1:A:399:HIS:O	1:A:435:HIS:CD2	2.59	0.54
2:B:856:PHE:CE1	2:B:969:ARG:HG3	2.42	0.54
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.89	0.54
1:A:754:SER:H	1:A:757:ASN:ND2	2.05	0.54
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.54	0.54
2:B:443:ASN:HD22	2:B:446:LEU:H	1.54	0.54
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.88	0.54
1:A:1292:PRO:HA	1:A:1298:TYR:HA	1.89	0.54
2:B:110:HIS:NE2	12:L:54:ARG:NH1	2.55	0.54
10:J:6:ARG:H	10:J:14:VAL:H	1.56	0.54
1:A:265:LYS:HZ1	1:A:299:HIS:CD2	2.25	0.54
8:H:104:PHE:CE1	8:H:136:LYS:HA	2.43	0.54
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.42	0.54
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.08	0.54
3:C:15:LYS:NZ	3:C:135:GLN:HG2	2.22	0.54
2:B:786:ASN:HA	2:B:967:ARG:HH22	1.73	0.54
1:A:714:PHE:O	1:A:718:VAL:HG23	2.08	0.54
13:M:35:VAL:HG22	13:M:46:ALA:HB2	1.89	0.54
1:A:1120:LEU:CD1	1:A:1125:ALA:HA	2.38	0.54
2:B:654:ARG:H	2:B:657:HIS:HD2	1.56	0.54
2:B:102:VAL:HG23	2:B:112:LEU:HD22	1.88	0.54
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.72	0.54
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.06	0.54
1:A:503:GLN:HE22	6:F:90:ARG:HH21	1.55	0.54
1:A:34:LYS:HB2	1:A:57:ARG:HH12	1.72	0.53
3:C:66:ARG:CZ	10:J:2:ILE:HG23	2.38	0.53
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.88	0.53
10:J:1:MET:H2	10:J:56:LEU:N	2.06	0.53
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.89	0.53
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.74	0.53
2:B:1147:LEU:HD22	2:B:1151:LEU:CD2	2.38	0.53
2:B:653:VAL:HG22	2:B:689:LEU:HB2	1.91	0.53
1:A:46:THR:HG22	1:A:47:ARG:H	1.72	0.53
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.89	0.53
1:A:412:ARG:HH12	2:B:1108:ARG:HD2	1.74	0.53
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.91	0.53
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.90	0.53
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:135:LEU:HB3	8:H:137:GLN:HG2	1.91	0.53
1:A:839:ARG:NH2	1:A:1402:PHE:HA	2.23	0.53
1:A:417:TYR:HB2	13:M:49:GLY:HA2	1.90	0.53
11:K:65:HIS:HD2	11:K:67:PHE:N	1.93	0.53
7:G:14:HIS:CD2	7:G:16:SER:H	2.27	0.53
1:A:67:CYS:C	1:A:68:GLN:HG3	2.28	0.52
1:A:711:ARG:HE	9:I:97:MET:HG3	1.74	0.52
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.91	0.52
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.91	0.52
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.74	0.52
1:A:1005:GLU:HG3	1:A:1009:ASN:HD21	1.74	0.52
2:B:303:TYR:CD1	2:B:571:PRO:HB3	2.40	0.52
2:B:72:GLU:HB3	2:B:87:LYS:HG2	1.90	0.52
2:B:280:ILE:HG13	2:B:333:PHE:HE1	1.74	0.52
1:A:534:LEU:O	1:A:574:GLY:HA3	2.08	0.52
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.90	0.52
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.92	0.52
1:A:1400:CYS:HB2	1:A:1405:THR:HA	1.91	0.52
4:D:8:PHE:HD2	7:G:6:ASP:HB2	1.74	0.52
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.91	0.52
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.91	0.52
1:A:851:HIS:HB2	1:A:855:THR:HG22	1.92	0.52
4:D:51:ASN:O	4:D:54:GLU:HB3	2.09	0.52
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.49	0.52
1:A:56:PRO:O	1:A:57:ARG:CD	2.58	0.52
13:M:136:LEU:HD21	13:M:196:ILE:HB	1.92	0.52
3:C:66:ARG:NH2	10:J:3:VAL:O	2.40	0.52
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.92	0.52
1:A:1129:GLU:HA	1:A:1132:LYS:HD2	1.92	0.51
4:D:12:ARG:HD3	4:D:14:ARG:HG2	1.92	0.51
7:G:125:SER:HB2	7:G:131:GLN:HE22	1.75	0.51
1:A:332:LYS:O	1:A:333:GLU:HB2	2.10	0.51
7:G:1:MET:HE2	7:G:3:PHE:CD1	2.46	0.51
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.19	0.51
2:B:424:LEU:HD22	2:B:453:ILE:HD11	1.92	0.51
2:B:335:GLY:HA3	2:B:348:ARG:HB2	1.91	0.51
1:A:535:THR:O	1:A:575:LYS:HE2	2.11	0.51
1:A:347:PHE:CE1	2:B:1107:ALA:HB1	2.46	0.51
1:A:709:THR:HG23	9:I:94:ASP:HA	1.92	0.51
10:J:1:MET:H2	10:J:57:ILE:H	1.58	0.51
10:J:6:ARG:HG3	10:J:13:VAL:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:SER:O	1:A:919:ILE:HB	2.11	0.51
2:B:900:ALA:HA	12:L:58:LYS:HD3	1.93	0.51
2:B:957:ASN:HD21	2:B:961:LEU:HD12	1.75	0.51
1:A:524:VAL:HG12	1:A:525:GLN:H	1.75	0.51
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.09	0.51
7:G:1:MET:HE2	7:G:2:PHE:N	2.25	0.50
2:B:361:LEU:HB3	2:B:364:ILE:HD12	1.93	0.50
13:M:114:GLN:O	13:M:118:VAL:HG23	2.10	0.50
2:B:486:TYR:HB3	2:B:1096:ARG:HH12	1.76	0.50
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.93	0.50
2:B:806:THR:HB	2:B:809:MET:HG3	1.92	0.50
3:C:37:MET:HA	3:C:41:ILE:HD12	1.92	0.50
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.51	0.50
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.26	0.50
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.76	0.50
1:A:42:ASP:O	1:A:44:THR:N	2.37	0.50
1:A:146:MET:HA	1:A:171:GLN:HB2	1.93	0.50
1:A:1387:HIS:HA	1:A:1391:ARG:HG3	1.92	0.50
2:B:685:LEU:HD12	2:B:690:VAL:HG23	1.94	0.50
1:A:1188:GLN:HG2	1:A:1243:VAL:HG12	1.94	0.50
1:A:31:SER:HA	1:A:81:PHE:O	2.11	0.50
2:B:642:ASP:HA	2:B:649:LYS:HA	1.93	0.50
2:B:284:ILE:HG21	2:B:333:PHE:CD1	2.47	0.50
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.93	0.49
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.94	0.49
2:B:90:ILE:HD11	2:B:134:LYS:HZ3	1.77	0.49
1:A:626:ASN:O	1:A:631:HIS:HD2	1.95	0.49
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.94	0.49
10:J:36:LEU:HD11	10:J:51:LEU:HD13	1.94	0.49
2:B:209:GLU:OE1	2:B:788:ARG:NH2	2.43	0.49
3:C:73:GLN:NE2	3:C:75:MET:H	2.06	0.49
2:B:744:HIS:CD2	2:B:746:SER:H	2.26	0.49
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.10	0.49
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.45	0.49
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.47	0.49
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.94	0.49
1:A:321:PRO:HD2	13:M:73:GLY:HA3	1.94	0.49
2:B:70:ILE:CG2	2:B:89:GLU:HG2	2.42	0.49
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.95	0.49
5:E:56:LYS:HE2	5:E:84:ASP:H	1.77	0.49
1:A:332:LYS:HB2	1:A:337:ARG:CZ	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.93	0.48
13:M:123:ASP:HA	13:M:126:VAL:HB	1.95	0.48
1:A:34:LYS:H	1:A:57:ARG:HH11	1.60	0.48
6:F:118:LEU:O	6:F:122:MET:HG3	2.13	0.48
2:B:373:ARG:HG3	2:B:567:GLU:HG2	1.95	0.48
8:H:6:PHE:CD1	8:H:130:ARG:HG2	2.46	0.48
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.95	0.48
1:A:42:ASP:C	1:A:44:THR:H	2.17	0.48
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.96	0.48
13:M:199:LYS:HB2	13:M:202:GLU:HB3	1.95	0.48
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.95	0.48
2:B:648:HIS:CD2	2:B:649:LYS:H	2.31	0.48
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.96	0.48
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.96	0.48
6:F:76:LYS:O	6:F:79:ARG:HD3	2.13	0.48
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.94	0.48
1:A:86:LEU:HD11	1:A:239:LEU:HD13	1.96	0.48
3:C:22:LEU:HD11	11:K:101:LEU:HD21	1.96	0.48
1:A:715:GLU:O	1:A:719:VAL:HG23	2.14	0.48
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.48	0.48
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.96	0.48
1:A:596:THR:C	1:A:598:LEU:H	2.16	0.48
2:B:515:HIS:HD2	2:B:517:THR:N	1.89	0.48
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.95	0.47
1:A:180:LYS:HA	1:A:180:LYS:HE2	1.96	0.47
1:A:121:LEU:HB2	1:A:141:LEU:HD21	1.95	0.47
10:J:1:MET:N	10:J:56:LEU:N	2.61	0.47
4:D:14:ARG:C	4:D:16:LYS:H	2.18	0.47
1:A:1387:HIS:HB3	1:A:1391:ARG:NH2	2.29	0.47
12:L:31:CYS:O	12:L:35:SER:HA	2.14	0.47
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.96	0.47
2:B:956:THR:HA	2:B:961:LEU:O	2.13	0.47
2:B:25:ILE:HG21	2:B:658:ILE:HD13	1.97	0.47
2:B:54:PHE:HA	2:B:58:THR:HB	1.97	0.47
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.50	0.47
5:E:80:VAL:HG22	5:E:109:ILE:HB	1.97	0.47
1:A:66:LYS:NZ	1:A:68:GLN:H	2.13	0.47
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.97	0.47
2:B:44:VAL:HA	2:B:46:GLN:HE21	1.80	0.47
2:B:603:LEU:HB3	2:B:609:ILE:HG23	1.95	0.47
1:A:416:ARG:HH22	13:M:40:GLU:HG2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:LYS:CB	2:B:471:LYS:HB2	2.37	0.47
1:A:320:ARG:NH2	13:M:80:GLY:O	2.47	0.47
3:C:241:ASP:HB3	11:K:109:TRP:CD2	2.49	0.47
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.79	0.47
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.95	0.47
6:F:154:ASP:H	6:F:155:LEU:HD12	1.79	0.47
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.96	0.47
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.80	0.47
2:B:818:PRO:HG2	10:J:54:VAL:HG21	1.96	0.47
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.97	0.47
1:A:745:GLN:HA	1:A:748:MET:HE3	1.97	0.46
6:F:155:LEU:CD1	6:F:155:LEU:H	2.25	0.46
2:B:493:SER:OG	2:B:526:GLU:OE2	2.32	0.46
1:A:756:ILE:HG22	1:A:760:GLN:HE21	1.80	0.46
10:J:53:HIS:HE1	10:J:55:ASP:OD1	1.99	0.46
3:C:142:VAL:HG11	10:J:5:VAL:HG13	1.97	0.46
2:B:273:LEU:HD23	2:B:274:PRO:HD2	1.98	0.46
1:A:42:ASP:C	1:A:44:THR:N	2.69	0.46
2:B:1150:ARG:HA	2:B:1154:ALA:HB3	1.98	0.46
4:D:17:LYS:HD2	4:D:18:VAL:H	1.81	0.46
1:A:1031:VAL:HA	1:A:1035:TYR:HD2	1.80	0.46
2:B:333:PHE:O	2:B:337:ARG:HD2	2.14	0.46
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.50	0.46
1:A:440:ASP:O	1:A:460:VAL:HG23	2.15	0.46
2:B:294:ASP:H	9:I:12:ASN:HD22	1.61	0.46
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.51	0.46
8:H:130:ARG:N	8:H:130:ARG:HD3	2.24	0.46
2:B:516:ASN:ND2	2:B:516:ASN:H	2.10	0.46
1:A:579:SER:HB3	1:A:611:GLN:HA	1.97	0.46
2:B:468:GLU:HB2	2:B:471:LYS:HD3	1.96	0.46
1:A:568:PRO:HB2	3:C:221:TYR:CE2	2.51	0.46
2:B:1009:ASP:OD2	10:J:48:ARG:NH2	2.48	0.46
2:B:106:ASP:HA	13:M:186:ALA:HB3	1.96	0.46
11:K:56:VAL:HA	11:K:77:THR:HG22	1.97	0.46
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.16	0.46
2:B:338:GLY:HA3	2:B:351:TYR:HE2	1.80	0.46
1:A:33:ALA:HA	1:A:57:ARG:HD3	1.98	0.46
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.46	0.46
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.46	0.46
1:A:915:SER:HB2	1:A:919:ILE:HD13	1.97	0.46
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:652:LYS:HD2	2:B:688:GLY:O	2.15	0.46
6:F:99:LEU:O	6:F:103:MET:HG2	2.16	0.46
1:A:1327:ILE:O	5:E:147:HIS:HE1	1.99	0.46
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.97	0.46
7:G:106:MET:HG2	7:G:107:LYS:N	2.30	0.45
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.97	0.45
1:A:68:GLN:O	1:A:70:CYS:N	2.45	0.45
3:C:6:PRO:HB2	11:K:101:LEU:HG	1.98	0.45
7:G:115:MET:HG3	7:G:163:ILE:HD11	1.98	0.45
1:A:344:ARG:HD2	2:B:1119:VAL:O	2.16	0.45
2:B:435:THR:HG23	2:B:442:PHE:HD1	1.81	0.45
1:A:845:LEU:HA	1:A:848:ILE:CD1	2.47	0.45
1:A:508:PRO:HB2	1:A:639:PRO:HB2	1.98	0.45
1:A:567:LYS:NZ	8:H:91:ASP:HA	2.32	0.45
13:M:143:PRO:HG3	13:M:185:VAL:HG21	1.98	0.45
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.50	0.45
7:G:91:VAL:CG2	7:G:143:ILE:HD13	2.46	0.45
2:B:800:GLN:CB	10:J:52:THR:HG22	2.47	0.45
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.97	0.45
2:B:1081:LEU:O	3:C:189:THR:HG23	2.17	0.45
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.98	0.45
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.97	0.45
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.98	0.45
2:B:211:VAL:O	2:B:480:SER:HA	2.16	0.45
1:A:109:HIS:H	1:A:210:ILE:HG12	1.82	0.45
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.64	0.45
2:B:903:VAL:HG23	12:L:61:THR:HG21	1.99	0.45
2:B:283:VAL:HG13	2:B:297:ILE:HD13	1.99	0.45
1:A:356:ASP:OD2	1:A:469:ARG:HD3	2.17	0.44
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.00	0.44
1:A:708:MET:HG2	1:A:712:GLU:HB3	1.99	0.44
1:A:786:HIS:HA	2:B:703:ILE:O	2.17	0.44
1:A:416:ARG:NH2	13:M:40:GLU:HG2	2.32	0.44
1:A:705:LYS:NZ	1:A:716:ASP:OD2	2.51	0.44
4:D:52:LEU:O	4:D:53:SER:CB	2.65	0.44
1:A:856:THR:HB	1:A:865:GLN:HB2	1.99	0.44
1:A:34:LYS:H	1:A:57:ARG:NH1	2.15	0.44
11:K:16:GLU:OE1	11:K:37:LYS:HE3	2.17	0.44
1:A:323:LYS:HE3	13:M:76:PRO:HA	1.99	0.44
1:A:850:VAL:CG2	1:A:1064:VAL:HG21	2.45	0.44
1:A:754:SER:H	1:A:757:ASN:HD22	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:LYS:HD2	4:D:18:VAL:HG13	2.00	0.44
7:G:165:GLU:HG2	7:G:168:LEU:HD12	2.00	0.44
1:A:564:ALA:N	1:A:576:GLN:HE22	2.16	0.44
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.99	0.44
1:A:71:GLN:O	1:A:73:GLY:N	2.51	0.44
1:A:1107:VAL:HG13	1:A:1332:PHE:HE1	1.83	0.44
5:E:12:LEU:HD21	5:E:55:ARG:HH21	1.83	0.44
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.53	0.44
1:A:524:VAL:HG12	1:A:525:GLN:HG2	2.00	0.44
2:B:276:ILE:HG23	2:B:337:ARG:HB3	2.00	0.44
1:A:512:VAL:HA	1:A:519:PRO:HA	1.99	0.44
5:E:78:LEU:HD21	5:E:109:ILE:HD12	2.00	0.44
1:A:605:MET:HG2	1:A:621:THR:HG21	2.00	0.44
7:G:10:ASN:HA	7:G:70:PHE:O	2.18	0.43
4:D:24:ALA:HB1	4:D:25:ALA:H	1.60	0.43
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.99	0.43
2:B:205:ILE:HD13	2:B:461:LEU:HB3	2.00	0.43
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.00	0.43
3:C:173:ALA:HB2	3:C:243:VAL:HG11	1.99	0.43
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.18	0.43
9:I:19:ASP:HB2	9:I:26:LEU:HD11	2.00	0.43
1:A:767:GLN:HA	1:A:799:PHE:HA	1.99	0.43
6:F:75:PRO:HG2	6:F:78:GLN:HB2	2.00	0.43
2:B:806:THR:HG22	2:B:808:ALA:H	1.82	0.43
4:D:23:ASN:HA	4:D:28:GLN:O	2.18	0.43
3:C:166:GLU:HG2	11:K:10:PHE:HZ	1.83	0.43
1:A:1445:ILE:HD11	7:G:68:ALA:CB	2.48	0.43
1:A:396:PRO:HB3	1:A:403:LYS:HA	1.99	0.43
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.19	0.43
1:A:260:ASP:OD1	1:A:328:ARG:NH2	2.45	0.43
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.49	0.43
4:D:52:LEU:O	4:D:53:SER:HB2	2.19	0.43
10:J:1:MET:N	10:J:56:LEU:H	2.16	0.43
1:A:265:LYS:CG	1:A:303:TYR:HB2	2.48	0.43
8:H:42:ILE:O	8:H:44:VAL:HG23	2.18	0.43
1:A:824:LEU:HD21	2:B:769:TYR:HE1	1.83	0.43
2:B:309:GLN:HG3	9:I:52:ILE:HD11	2.01	0.43
1:A:265:LYS:NZ	1:A:299:HIS:HD2	2.17	0.43
11:K:61:TYR:HA	11:K:72:LYS:O	2.19	0.43
4:D:168:LYS:HA	4:D:168:LYS:HD2	1.88	0.43
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:23:VAL:HA	8:H:42:ILE:O	2.19	0.43
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.53	0.43
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.01	0.43
1:A:51:GLY:C	1:A:56:PRO:HB3	2.39	0.43
1:A:369:SER:HB3	11:K:2:ASN:ND2	2.32	0.43
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	2.00	0.43
3:C:166:GLU:HG2	11:K:10:PHE:CZ	2.53	0.43
1:A:919:ILE:HG12	1:A:983:ILE:HD13	2.00	0.42
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.01	0.42
11:K:81:TYR:OH	11:K:86:ALA:HA	2.19	0.42
1:A:202:LEU:HB3	1:A:207:ILE:HD11	2.00	0.42
5:E:151:PRO:HD2	5:E:153:HIS:HE1	1.83	0.42
1:A:1170:ILE:H	1:A:1170:ILE:HG13	1.62	0.42
2:B:597:MET:HA	2:B:600:LEU:HD12	2.00	0.42
4:D:53:SER:HB3	4:D:154:PHE:O	2.19	0.42
8:H:80:ARG:HG2	11:K:57:LEU:HD22	2.00	0.42
12:L:40:LEU:HD11	12:L:49:LYS:NZ	2.34	0.42
1:A:845:LEU:HA	1:A:848:ILE:HD12	2.01	0.42
7:G:91:VAL:HG23	7:G:143:ILE:HD13	2.00	0.42
7:G:43:GLY:HA2	7:G:157:ILE:HD11	2.00	0.42
1:A:1225:PHE:H	1:A:1242:VAL:H	1.67	0.42
1:A:356:ASP:OD2	11:K:65:HIS:HE1	2.02	0.42
1:A:1311:VAL:HG21	1:A:1329:THR:HG23	2.02	0.42
2:B:123:THR:HG23	2:B:205:ILE:HA	2.01	0.42
1:A:573:SER:O	1:A:576:GLN:HB3	2.19	0.42
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.01	0.42
1:A:535:THR:HG21	1:A:617:VAL:H	1.84	0.42
2:B:684:LEU:HB3	2:B:690:VAL:HG22	2.00	0.42
2:B:134:LYS:HZ1	2:B:442:PHE:HB2	1.85	0.42
2:B:976:ILE:HD11	2:B:992:ILE:HA	2.01	0.42
1:A:1220:PHE:HE2	1:A:1271:ILE:HD11	1.84	0.42
2:B:751:VAL:HG13	2:B:812:LEU:HD22	2.01	0.42
7:G:111:THR:C	7:G:113:HIS:H	2.23	0.42
10:J:25:LEU:O	10:J:29:GLU:HA	2.19	0.42
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.00	0.42
4:D:167:LEU:HB3	4:D:177:VAL:HG12	2.01	0.42
2:B:1181:GLU:HG3	2:B:1188:LYS:HG2	2.02	0.42
1:A:116:ASP:HB3	1:A:118:HIS:H	1.84	0.42
3:C:15:LYS:HZ1	3:C:135:GLN:HG2	1.83	0.42
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.54	0.42
1:A:5:GLN:HG3	2:B:1175:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.20	0.42
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.54	0.42
1:A:197:PRO:HG2	1:A:199:LEU:HD11	2.01	0.42
2:B:758:PHE:CE2	2:B:1027:ILE:HG22	2.54	0.42
1:A:265:LYS:NZ	1:A:299:HIS:CD2	2.88	0.42
1:A:1140:HIS:CE1	1:A:1272:THR:HG23	2.54	0.42
2:B:1124:ARG:HG3	13:M:58:ASP:OD2	2.20	0.42
1:A:128:ILE:HB	1:A:134:ARG:HG3	2.01	0.42
12:L:61:THR:HB	12:L:63:ARG:CG	2.37	0.42
2:B:1181:GLU:HA	2:B:1187:ASN:O	2.20	0.42
2:B:786:ASN:HA	2:B:967:ARG:NH2	2.35	0.42
5:E:39:LEU:HG	5:E:43:LYS:HE2	2.02	0.42
1:A:800:VAL:HA	1:A:812:GLU:HG2	2.02	0.42
2:B:345:LYS:HG2	2:B:349:ILE:HD11	2.02	0.42
2:B:486:TYR:HA	2:B:1096:ARG:NH2	2.29	0.42
5:E:147:HIS:CD2	5:E:149:LEU:H	2.38	0.42
1:A:986:ILE:O	1:A:990:VAL:HG23	2.20	0.42
2:B:1057:LYS:HD2	2:B:1058:LEU:HD23	2.02	0.42
2:B:69:LEU:HD22	2:B:425:THR:HG23	2.01	0.42
9:I:5:ARG:HG3	9:I:14:LEU:HD12	2.02	0.42
1:A:46:THR:HG22	1:A:47:ARG:N	2.34	0.41
6:F:116:ASP:HB3	6:F:119:ARG:HB2	2.02	0.41
2:B:1202:LEU:HA	2:B:1202:LEU:HD22	1.94	0.41
3:C:65:HIS:CE1	3:C:69:LEU:HD11	2.55	0.41
1:A:1442:ASP:HB2	6:F:137:TYR:CE2	2.46	0.41
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.55	0.41
1:A:320:ARG:HH21	13:M:78:ARG:NH2	2.18	0.41
2:B:269:ILE:HD12	2:B:317:CYS:SG	2.61	0.41
1:A:599:SER:HA	1:A:600:PRO:HD2	1.96	0.41
2:B:515:HIS:H	2:B:518:HIS:HD2	1.63	0.41
1:A:1005:GLU:HG3	1:A:1009:ASN:ND2	2.33	0.41
5:E:46:TYR:HD1	5:E:57:MET:HB3	1.85	0.41
2:B:843:GLN:HA	2:B:846:ILE:HD12	2.02	0.41
5:E:88:VAL:HB	5:E:116:ILE:HA	2.02	0.41
2:B:175:ARG:HB2	2:B:200:GLY:HA3	2.01	0.41
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.54	0.41
3:C:73:GLN:HE21	3:C:75:MET:N	2.09	0.41
3:C:164:ALA:HA	3:C:167:HIS:O	2.21	0.41
2:B:102:VAL:HG21	2:B:122:LEU:HD13	2.02	0.41
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.02	0.41
2:B:555:ILE:HA	2:B:558:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LEU:HD12	3:C:145:CYS:HB2	2.01	0.41
7:G:1:MET:HE1	7:G:80:LYS:N	2.32	0.41
1:A:337:ARG:NH1	2:B:1132:GLU:OE1	2.51	0.41
1:A:774:ARG:HB2	1:A:797:LYS:HB3	2.03	0.41
2:B:1048:THR:HB	2:B:1050:ILE:HD12	2.03	0.41
2:B:428:ILE:O	2:B:432:MET:HG3	2.20	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.21	0.41
1:A:287:HIS:HA	1:A:290:GLU:CD	2.40	0.41
1:A:597:LEU:HD13	1:A:597:LEU:HA	1.90	0.41
2:B:859:TYR:OH	2:B:942:ARG:HG2	2.21	0.41
1:A:72:GLU:HB3	1:A:76:GLU:HB3	2.01	0.41
13:M:160:GLU:HG3	13:M:213:ILE:HD13	2.03	0.41
3:C:259:LEU:HD13	11:K:91:CYS:HB2	2.01	0.41
9:I:77:LYS:HB2	9:I:108:HIS:CD2	2.56	0.41
10:J:48:ARG:O	10:J:52:THR:HB	2.21	0.41
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	2.02	0.41
1:A:844:ALA:HA	1:A:1389:PHE:CD2	2.56	0.41
7:G:127:PRO:HD2	7:G:138:THR:HG21	2.03	0.41
8:H:130:ARG:CD	8:H:130:ARG:H	2.14	0.41
1:A:626:ASN:O	1:A:631:HIS:CD2	2.74	0.41
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	2.02	0.41
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.56	0.41
3:C:169:LYS:HE3	3:C:170:TRP:CH2	2.56	0.41
12:L:27:LEU:HA	12:L:39:SER:HB2	2.01	0.41
2:B:658:ILE:HA	2:B:661:LEU:HD12	2.02	0.41
2:B:106:ASP:O	2:B:108:VAL:N	2.54	0.41
4:D:23:ASN:HB3	7:G:82:PHE:HD1	1.86	0.41
2:B:841:MET:HB3	2:B:993:THR:HG22	2.03	0.41
4:D:68:ARG:HB2	4:D:72:ARG:HH21	1.86	0.41
7:G:15:PRO:HD3	7:G:67:SER:HA	2.03	0.41
3:C:252:GLN:HG2	11:K:95:ILE:HG23	2.03	0.41
5:E:86:PRO:HA	5:E:113:GLN:HB2	2.03	0.41
1:A:465:TYR:CE1	11:K:4:PRO:HD3	2.56	0.41
2:B:311:LEU:HB3	9:I:4:PHE:CZ	2.56	0.41
1:A:567:LYS:HZ2	8:H:91:ASP:HA	1.86	0.41
2:B:199:MET:N	2:B:199:MET:SD	2.84	0.41
2:B:816:GLU:C	2:B:818:PRO:HD3	2.41	0.40
10:J:7:CYS:HA	10:J:49:MET:HG2	2.02	0.40
11:K:7:PHE:C	11:K:9:LEU:H	2.24	0.40
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.93	0.40
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.49	0.40
4:D:52:LEU:HB3	4:D:148:LEU:CD2	2.49	0.40
2:B:47:GLN:HE21	2:B:408:LEU:HD23	1.85	0.40
3:C:20:PHE:HE2	3:C:22:LEU:HD13	1.87	0.40
1:A:709:THR:HG22	1:A:711:ARG:H	1.84	0.40
1:A:265:LYS:NZ	13:M:94:THR:OG1	2.52	0.40
2:B:1159:ARG:HG3	2:B:1195:HIS:CE1	2.56	0.40
1:A:521:MET:C	1:A:624:SER:HB3	2.42	0.40
2:B:466:TRP:HB2	2:B:479:VAL:HG21	2.02	0.40
5:E:147:HIS:HB3	5:E:150:VAL:HG23	2.03	0.40
1:A:928:LEU:HD22	1:A:987:VAL:HG11	2.02	0.40
3:C:176:ILE:HG12	3:C:232:VAL:HG13	2.04	0.40
2:B:283:VAL:HG22	2:B:297:ILE:HG21	2.04	0.40
2:B:74:LEU:HA	2:B:85:SER:HA	2.04	0.40
3:C:93:ASP:O	3:C:127:ARG:NH2	2.55	0.40
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	2.03	0.40
2:B:256:VAL:HG12	2:B:385:LEU:HD22	2.02	0.40
2:B:1085:ILE:N	2:B:1085:ILE:HD12	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1404/1733 (81%)	1248 (89%)	107 (8%)	49 (4%)	4	35
2	B	1134/1224 (93%)	1007 (89%)	94 (8%)	33 (3%)	6	40
3	C	264/318 (83%)	239 (90%)	22 (8%)	3 (1%)	17	61
4	D	174/221 (79%)	152 (87%)	16 (9%)	6 (3%)	5	36
5	E	212/215 (99%)	196 (92%)	14 (7%)	2 (1%)	21	65
6	F	85/155 (55%)	79 (93%)	4 (5%)	2 (2%)	7	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	169/171 (99%)	151 (89%)	14 (8%)	4 (2%)	7	44
8	H	130/146 (89%)	110 (85%)	14 (11%)	6 (5%)	3	26
9	I	117/122 (96%)	96 (82%)	19 (16%)	2 (2%)	11	51
10	J	63/70 (90%)	54 (86%)	6 (10%)	3 (5%)	3	25
11	K	112/120 (93%)	107 (96%)	4 (4%)	1 (1%)	21	65
12	L	42/70 (60%)	28 (67%)	12 (29%)	2 (5%)	3	25
13	M	191/345 (55%)	176 (92%)	12 (6%)	3 (2%)	12	53
All	All	4097/4910 (83%)	3643 (89%)	338 (8%)	116 (3%)	6	41

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	72	GLU
1	A	74	MET
1	A	254	GLU
1	A	317	LYS
1	A	330	LYS
1	A	424	ILE
1	A	466	SER
1	A	626	ASN
1	A	629	LEU
1	A	885	THR
1	A	1064	VAL
1	A	1122	PRO
1	A	1405	THR
2	B	107	GLY
2	B	251	ILE
2	B	369	GLY
2	B	531	GLN
2	B	708	GLU
2	B	733	HIS
2	B	1066	SER
4	D	18	VAL
7	G	154	VAL
7	G	155	SER
8	H	82	PRO
8	H	139	ASN
10	J	2	ILE

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Mol	Chain	Res	Type
13	M	197	HIS
1	A	66	LYS
1	A	68	GLN
1	A	252	PHE
1	A	333	GLU
1	A	775	ILE
1	A	884	ASP
2	B	108	VAL
2	B	471	LYS
2	B	643	ASP
2	B	723	VAL
2	B	1046	PRO
2	B	1156	ASP
2	B	1157	ALA
2	B	1221	SER
3	C	215	GLU
4	D	5	THR
4	D	199	ASN
5	E	3	GLN
6	F	78	GLN
7	G	139	ILE
8	H	18	GLY
9	I	57	GLY
12	L	45	ALA
12	L	50	ASP
1	A	62	ASP
1	A	69	THR
1	A	71	GLN
1	A	167	CYS
1	A	286	HIS
1	A	517	ASN
1	A	543	LEU
1	A	593	GLU
1	A	1206	ASP
1	A	1242	VAL
1	A	1255	GLU
1	A	1377	THR
1	A	1403	GLU
2	B	229	ALA
2	B	266	ALA
2	B	440	HIS
2	B	466	TRP

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Mol	Chain	Res	Type
2	B	629	ASP
2	B	792	MET
2	B	992	ILE
3	C	90	ASP
4	D	4	SER
6	F	104	ASN
8	H	17	PRO
8	H	86	ASP
9	I	105	SER
13	M	167	SER
1	A	31	SER
1	A	948	VAL
1	A	1365	TYR
2	B	230	ALA
2	B	245	GLU
2	B	711	GLU
2	B	1155	SER
2	B	1223	ASP
4	D	14	ARG
4	D	198	LEU
7	G	112	LYS
10	J	6	ARG
13	M	200	THR
1	A	42	ASP
1	A	44	THR
1	A	399	HIS
1	A	465	TYR
1	A	597	LEU
1	A	599	SER
1	A	958	VAL
1	A	1280	GLU
2	B	247	GLY
2	B	441	ASP
2	B	809	MET
2	B	1181	GLU
2	B	1222	ARG
5	E	36	GLU
11	K	26	LYS
1	A	196	GLU
2	B	250	PHE
8	H	130	ARG
1	A	52	GLY

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Mol	Chain	Res	Type
3	C	105	GLY
1	A	35	ILE
10	J	64	ASN
1	A	51	GLY

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	1236/1520 (81%)	1063 (86%)	173 (14%)	4	23
2	B	980/1061 (92%)	835 (85%)	145 (15%)	4	20
3	C	234/274 (85%)	203 (87%)	31 (13%)	5	25
4	D	160/200 (80%)	129 (81%)	31 (19%)	2	8
5	E	196/197 (100%)	176 (90%)	20 (10%)	9	38
6	F	77/137 (56%)	69 (90%)	8 (10%)	9	37
7	G	152/152 (100%)	134 (88%)	18 (12%)	6	29
8	H	118/128 (92%)	98 (83%)	20 (17%)	2	14
9	I	113/116 (97%)	101 (89%)	12 (11%)	8	36
10	J	60/65 (92%)	48 (80%)	12 (20%)	1	8
11	K	99/102 (97%)	87 (88%)	12 (12%)	6	28
12	L	39/57 (68%)	31 (80%)	8 (20%)	1	7
13	M	142/299 (48%)	109 (77%)	33 (23%)	1	4
All	All	3606/4308 (84%)	3083 (86%)	523 (14%)	4	21

All (523) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	13	THR
1	A	15	LYS
1	A	28	ARG

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Mol	Chain	Res	Type
1	A	36	ARG
1	A	41	MET
1	A	42	ASP
1	A	43	GLU
1	A	45	GLN
1	A	47	ARG
1	A	53	LEU
1	A	57	ARG
1	A	62	ASP
1	A	64	ASN
1	A	66	LYS
1	A	68	GLN
1	A	70	CYS
1	A	74	MET
1	A	85	ASP
1	A	93	VAL
1	A	98	LYS
1	A	109	HIS
1	A	113	LEU
1	A	131	SER
1	A	141	LEU
1	A	145	LYS
1	A	146	MET
1	A	149	GLU
1	A	151	ASP
1	A	159	THR
1	A	160	GLN
1	A	167	CYS
1	A	196	GLU
1	A	200	ARG
1	A	204	THR
1	A	220	THR
1	A	237	THR
1	A	249	SER
1	A	250	ILE
1	A	257	ARG
1	A	265	LYS
1	A	277	GLU
1	A	279	LEU
1	A	302	THR
1	A	303	TYR
1	A	307	ASP

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	335	ARG
1	A	344	ARG
1	A	369	SER
1	A	375	THR
1	A	385	ILE
1	A	397	ASN
1	A	408	ASP
1	A	419	LYS
1	A	420	ARG
1	A	425	GLN
1	A	434	ARG
1	A	443	LEU
1	A	444	PHE
1	A	451	HIS
1	A	470	LEU
1	A	475	THR
1	A	476	SER
1	A	493	GLN
1	A	504	LEU
1	A	516	SER
1	A	527	THR
1	A	566	ILE
1	A	567	LYS
1	A	571	LEU
1	A	577	ILE
1	A	597	LEU
1	A	603	ASN
1	A	609	ASP
1	A	618	GLU
1	A	621	THR
1	A	622	VAL
1	A	626	ASN
1	A	629	LEU
1	A	634	THR
1	A	644	LYS
1	A	652	VAL
1	A	666	ILE
1	A	670	ILE
1	A	685	GLU
1	A	691	LEU
1	A	722	LEU

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Mol	Chain	Res	Type
1	A	732	LEU
1	A	739	ASP
1	A	756	ILE
1	A	768	GLN
1	A	769	SER
1	A	774	ARG
1	A	782	ARG
1	A	795	GLU
1	A	801	GLU
1	A	805	LEU
1	A	821	ARG
1	A	830	LYS
1	A	834	THR
1	A	855	THR
1	A	880	LYS
1	A	882	SER
1	A	884	ASP
1	A	886	ILE
1	A	896	ARG
1	A	898	ARG
1	A	905	ASP
1	A	915	SER
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	924	LYS
1	A	931	GLU
1	A	940	ARG
1	A	973	ILE
1	A	976	THR
1	A	991	LYS
1	A	992	ASP
1	A	998	LEU
1	A	1001	ARG
1	A	1029	ARG
1	A	1030	ARG
1	A	1038	THR
1	A	1047	SER
1	A	1052	GLN
1	A	1058	VAL
1	A	1064	VAL
1	A	1081	LEU

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Mol	Chain	Res	Type
1	A	1093	LYS
1	A	1110	ASN
1	A	1113	THR
1	A	1116	LEU
1	A	1120	LEU
1	A	1142	THR
1	A	1147	THR
1	A	1159	ARG
1	A	1163	ILE
1	A	1170	ILE
1	A	1171	GLN
1	A	1195	LEU
1	A	1196	GLU
1	A	1203	ASN
1	A	1217	LYS
1	A	1218	GLN
1	A	1222	ASN
1	A	1230	GLU
1	A	1237	ILE
1	A	1257	ASP
1	A	1259	MET
1	A	1260	LEU
1	A	1264	GLU
1	A	1267	MET
1	A	1273	LEU
1	A	1274	ARG
1	A	1280	GLU
1	A	1297	GLU
1	A	1299	VAL
1	A	1308	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1366	ARG
1	A	1370	LEU
1	A	1400	CYS
1	A	1405	THR
1	A	1406	VAL
1	A	1422	ARG
1	A	1424	VAL
1	A	1426	GLU
1	A	1433	MET
1	A	1444	MET

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Mol	Chain	Res	Type
1	A	1445	ILE
2	B	26	THR
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	69	LEU
2	B	72	GLU
2	B	73	GLN
2	B	101	MET
2	B	103	ASN
2	B	104	GLU
2	B	128	LEU
2	B	175	ARG
2	B	178	ASN
2	B	183	GLU
2	B	199	MET
2	B	211	VAL
2	B	216	GLU
2	B	217	ARG
2	B	218	SER
2	B	223	VAL
2	B	227	LYS
2	B	228	LYS
2	B	232	SER
2	B	240	ILE
2	B	244	LEU
2	B	245	GLU
2	B	249	ARG
2	B	254	LEU
2	B	273	LEU
2	B	298	LEU
2	B	309	GLN
2	B	313	MET
2	B	323	VAL
2	B	331	LEU
2	B	337	ARG
2	B	358	LYS
2	B	367	LEU
2	B	371	GLU
2	B	384	ARG
2	B	387	LEU
2	B	391	ASP

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Mol	Chain	Res	Type
2	B	394	ASP
2	B	408	LEU
2	B	416	LEU
2	B	419	THR
2	B	425	THR
2	B	440	HIS
2	B	442	PHE
2	B	471	LYS
2	B	476	ARG
2	B	479	VAL
2	B	480	SER
2	B	485	ARG
2	B	490	SER
2	B	495	LEU
2	B	496	ARG
2	B	502	ILE
2	B	531	GLN
2	B	541	LEU
2	B	544	CYS
2	B	547	VAL
2	B	549	THR
2	B	574	SER
2	B	589	VAL
2	B	596	LEU
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG
2	B	609	ILE
2	B	610	ASN
2	B	616	ILE
2	B	620	ARG
2	B	621	GLU
2	B	623	GLU
2	B	625	LYS
2	B	628	THR
2	B	637	LEU
2	B	651	LEU
2	B	658	ILE
2	B	685	LEU
2	B	689	LEU
2	B	694	ASP
2	B	706	GLN

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Mol	Chain	Res	Type
2	B	710	LEU
2	B	733	HIS
2	B	736	THR
2	B	764	SER
2	B	766	ARG
2	B	786	ASN
2	B	805	THR
2	B	812	LEU
2	B	813	LYS
2	B	835	GLN
2	B	838	SER
2	B	853	SER
2	B	868	MET
2	B	879	ARG
2	B	883	LEU
2	B	906	SER
2	B	934	LYS
2	B	935	ARG
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	946	ASN
2	B	958	GLN
2	B	959	ASP
2	B	967	ARG
2	B	975	GLN
2	B	986	GLN
2	B	987	LYS
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1010	LEU
2	B	1028	GLU
2	B	1034	VAL
2	B	1056	SER
2	B	1057	LYS
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1094	ARG
2	B	1096	ARG
2	B	1108	ARG

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Mol	Chain	Res	Type
2	B	1111	MET
2	B	1113	VAL
2	B	1123	SER
2	B	1128	LEU
2	B	1135	ARG
2	B	1145	SER
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1160	VAL
2	B	1169	MET
2	B	1177	HIS
2	B	1182	CYS
2	B	1183	LYS
2	B	1189	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1216	LEU
2	B	1224	PHE
3	C	7	GLN
3	C	9	LYS
3	C	22	LEU
3	C	25	VAL
3	C	40	GLU
3	C	50	GLU
3	C	56	THR
3	C	74	SER
3	C	79	GLN
3	C	81	GLU
3	C	101	LEU
3	C	111	THR
3	C	121	VAL
3	C	127	ARG
3	C	129	ILE
3	C	145	CYS
3	C	149	LYS
3	C	156	THR
3	C	166	GLU
3	C	186	LEU
3	C	189	THR
3	C	199	LYS

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Mol	Chain	Res	Type
3	C	203	GLN
3	C	208	GLU
3	C	215	GLU
3	C	237	SER
3	C	240	VAL
3	C	260	LEU
3	C	263	THR
3	C	265	MET
3	C	268	ASP
4	D	8	PHE
4	D	11	ARG
4	D	12	ARG
4	D	13	ARG
4	D	15	LEU
4	D	16	LYS
4	D	17	LYS
4	D	19	GLU
4	D	22	GLU
4	D	31	GLN
4	D	34	GLN
4	D	35	LEU
4	D	41	GLN
4	D	47	LEU
4	D	48	ILE
4	D	51	ASN
4	D	52	LEU
4	D	65	GLU
4	D	118	THR
4	D	119	ARG
4	D	120	GLU
4	D	123	LEU
4	D	142	LYS
4	D	156	ASP
4	D	165	GLN
4	D	166	LEU
4	D	169	SER
4	D	177	VAL
4	D	200	ASN
4	D	201	LYS
4	D	203	SER
5	E	7	ARG
5	E	17	ARG

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Mol	Chain	Res	Type
5	E	25	ASP
5	E	31	THR
5	E	37	LEU
5	E	40	GLU
5	E	48	ASP
5	E	61	GLN
5	E	71	LYS
5	E	78	LEU
5	E	94	LYS
5	E	95	THR
5	E	100	ILE
5	E	102	GLU
5	E	107	THR
5	E	131	THR
5	E	159	ASP
5	E	165	LEU
5	E	173	SER
5	E	196	VAL
6	F	70	LYS
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	90	ARG
6	F	111	LEU
6	F	119	ARG
6	F	153	VAL
7	G	1	MET
7	G	2	PHE
7	G	13	LEU
7	G	22	MET
7	G	29	LYS
7	G	60	ARG
7	G	62	LEU
7	G	73	LYS
7	G	106	MET
7	G	111	THR
7	G	112	LYS
7	G	131	GLN
7	G	134	GLU
7	G	138	THR
7	G	139	ILE
7	G	141	SER

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Mol	Chain	Res	Type
7	G	143	ILE
7	G	165	GLU
8	H	3	ASN
8	H	11	GLN
8	H	19	ARG
8	H	27	GLU
8	H	32	THR
8	H	35	GLN
8	H	89	LEU
8	H	103	LYS
8	H	106	GLU
8	H	107	VAL
8	H	108	SER
8	H	110	ASP
8	H	111	LEU
8	H	112	ILE
8	H	124	ARG
8	H	129	TYR
8	H	130	ARG
8	H	131	ASN
8	H	135	LEU
8	H	136	LYS
9	I	5	ARG
9	I	17	ARG
9	I	21	GLU
9	I	50	THR
9	I	70	ARG
9	I	72	ASP
9	I	77	LYS
9	I	83	ASN
9	I	84	VAL
9	I	93	LYS
9	I	95	THR
9	I	114	GLN
10	J	2	ILE
10	J	6	ARG
10	J	13	VAL
10	J	14	VAL
10	J	20	SER
10	J	22	LEU
10	J	23	ASN
10	J	26	GLN

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Mol	Chain	Res	Type
10	J	38	ARG
10	J	42	LYS
10	J	48	ARG
10	J	57	ILE
11	K	14	GLU
11	K	20	LYS
11	K	25	THR
11	K	31	VAL
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	101	LEU
11	K	102	LYS
11	K	108	GLU
11	K	110	ASN
11	K	114	LEU
12	L	27	LEU
12	L	50	ASP
12	L	54	ARG
12	L	58	LYS
12	L	60	ARG
12	L	65	VAL
12	L	68	GLU
12	L	70	ARG
13	M	27	CYS
13	M	35	VAL
13	M	39	SER
13	M	47	LEU
13	M	48	CYS
13	M	51	VAL
13	M	52	LEU
13	M	56	LEU
13	M	59	THR
13	M	60	ARG
13	M	74	ASP
13	M	79	VAL
13	M	83	SER
13	M	84	ASN
13	M	86	LEU
13	M	88	ASP
13	M	90	ASN
13	M	93	SER

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Mol	Chain	Res	Type
13	M	101	THR
13	M	107	THR
13	M	119	MET
13	M	124	ASN
13	M	126	VAL
13	M	134	THR
13	M	136	LEU
13	M	142	LEU
13	M	145	ILE
13	M	158	HIS
13	M	168	MET
13	M	171	ILE
13	M	172	MET
13	M	182	ARG
13	M	209	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	68	GLN
1	A	83	HIS
1	A	171	GLN
1	A	281	HIS
1	A	282	ASN
1	A	299	HIS
1	A	339	ASN
1	A	394	ASN
1	A	425	GLN
1	A	435	HIS
1	A	503	GLN
1	A	517	ASN
1	A	631	HIS
1	A	741	ASN
1	A	757	ASN
1	A	760	GLN
1	A	768	GLN
1	A	854	ASN
1	A	858	ASN
1	A	903	ASN
1	A	965	GLN
1	A	969	GLN

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Mol	Chain	Res	Type
1	A	975	HIS
1	A	1232	ASN
1	A	1270	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	46	GLN
2	B	47	GLN
2	B	73	GLN
2	B	121	ASN
2	B	215	GLN
2	B	236	HIS
2	B	350	GLN
2	B	443	ASN
2	B	465	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	590	HIS
2	B	648	HIS
2	B	744	HIS
2	B	822	ASN
2	B	862	GLN
2	B	958	GLN
2	B	986	GLN
2	B	1015	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1161	HIS
2	B	1178	ASN
2	B	1193	GLN
2	B	1195	HIS
3	C	7	GLN
3	C	65	HIS
3	C	73	GLN
3	C	135	GLN
4	D	28	GLN
4	D	40	HIS
5	E	106	GLN
5	E	147	HIS
7	G	14	HIS

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Mol	Chain	Res	Type
7	G	131	GLN
8	H	131	ASN
9	I	12	ASN
9	I	83	ASN
10	J	53	HIS
11	K	29	ASN
11	K	65	HIS
12	L	53	HIS
12	L	66	GLN
13	M	84	ASN
13	M	117	ASN
13	M	124	ASN
13	M	158	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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, 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	1414/1733 (81%)	-0.06	28 (1%) 68 62	30, 65, 118, 185	0
2	B	1150/1224 (93%)	-0.08	46 (4%) 42 37	29, 69, 132, 191	0
3	C	266/318 (83%)	-0.14	2 (0%) 87 83	30, 53, 88, 140	0
4	D	178/221 (80%)	0.08	2 (1%) 82 77	43, 75, 120, 138	0
5	E	214/215 (99%)	0.35	16 (7%) 17 17	47, 101, 154, 173	0
6	F	87/155 (56%)	-0.26	0 100 100	32, 56, 88, 98	0
7	G	171/171 (100%)	-0.21	0 100 100	35, 56, 84, 104	0
8	H	134/146 (91%)	0.34	8 (5%) 25 23	55, 92, 134, 160	0
9	I	119/122 (97%)	0.24	8 (6%) 21 20	68, 98, 135, 166	0
10	J	65/70 (92%)	-0.43	0 100 100	35, 50, 76, 92	0
11	K	114/120 (95%)	-0.14	0 100 100	35, 56, 88, 100	0
12	L	44/70 (62%)	-0.02	1 (2%) 64 58	52, 90, 122, 136	0
13	M	193/345 (55%)	0.71	26 (13%) 4 4	52, 101, 140, 154	0
All	All	4149/4910 (84%)	-0.00	137 (3%) 50 45	29, 68, 132, 191	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	250	PHE	5.3
12	L	27	LEU	4.9
2	B	709	ASP	4.8
1	A	421	ALA	4.3
9	I	119	THR	4.3
5	E	50	MET	4.3
9	I	116	ASN	4.1
2	B	85	SER	4.1
2	B	643	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	140	ILE	4.0
13	M	123	ASP	4.0
9	I	120	GLN	3.9
2	B	79	THR	3.8
2	B	84	ILE	3.8
2	B	714	GLU	3.7
1	A	155	GLU	3.7
2	B	71	LEU	3.6
4	D	18	VAL	3.6
2	B	715	ALA	3.6
1	A	69	THR	3.5
5	E	126	SER	3.5
2	B	81	SER	3.5
13	M	178	ILE	3.5
2	B	137	TYR	3.5
1	A	159	THR	3.4
2	B	332	ASP	3.3
2	B	349	ILE	3.3
2	B	82	ASP	3.3
1	A	195	ASP	3.3
2	B	73	GLN	3.2
9	I	118	ARG	3.2
2	B	74	LEU	3.2
2	B	733	HIS	3.2
13	M	192	ILE	3.1
8	H	83	GLN	3.1
2	B	868	MET	3.1
1	A	1232	ASN	3.1
13	M	196	ILE	3.1
5	E	49	SER	3.1
1	A	161	LEU	3.1
1	A	422	GLY	3.1
1	A	154	SER	3.1
1	A	158	PRO	3.0
1	A	157	ASP	3.0
13	M	72	ASN	3.0
2	B	75	ALA	3.0
1	A	156	ASP	3.0
1	A	160	GLN	3.0
2	B	248	SER	3.0
13	M	198	VAL	3.0
13	M	171	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	77	HIS	2.9
13	M	71	HIS	2.9
9	I	115	LYS	2.9
2	B	88	TYR	2.9
2	B	328	GLU	2.8
2	B	78	THR	2.8
13	M	200	THR	2.8
8	H	86	ASP	2.8
8	H	132	LEU	2.8
9	I	60	GLN	2.7
2	B	139	ALA	2.7
5	E	93	MET	2.7
13	M	157	CYS	2.7
13	M	162	THR	2.7
2	B	86	ARG	2.7
13	M	203	PHE	2.7
2	B	722	ASP	2.6
13	M	209	ILE	2.6
13	M	204	GLY	2.6
2	B	72	GLU	2.5
2	B	136	THR	2.5
2	B	473	MET	2.5
5	E	53	PRO	2.5
13	M	197	HIS	2.5
8	H	85	GLY	2.5
1	A	1079	MET	2.5
2	B	70	ILE	2.5
5	E	88	VAL	2.5
2	B	134	LYS	2.5
1	A	973	ILE	2.4
9	I	114	GLN	2.4
3	C	268	ASP	2.4
1	A	64	ASN	2.4
2	B	346	GLU	2.4
2	B	345	LYS	2.4
5	E	40	GLU	2.4
2	B	334	ILE	2.4
13	M	159	ASP	2.4
5	E	66	GLU	2.3
5	E	39	LEU	2.3
5	E	42	PHE	2.3
1	A	151	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	83	ASN	2.3
8	H	131	ASN	2.3
13	M	168	MET	2.3
2	B	265	SER	2.3
2	B	90	ILE	2.3
1	A	1207	LEU	2.3
1	A	152	VAL	2.3
2	B	163	GLY	2.2
1	A	1124	HIS	2.2
2	B	138	GLU	2.2
2	B	666	TYR	2.2
1	A	150	THR	2.2
5	E	46	TYR	2.2
13	M	154	TYR	2.2
8	H	139	ASN	2.2
1	A	423	ASP	2.2
5	E	47	CYS	2.2
2	B	76	GLN	2.2
3	C	267	GLN	2.2
13	M	188	THR	2.2
5	E	96	PHE	2.2
13	M	153	ALA	2.2
13	M	177	LEU	2.2
4	D	221	TYR	2.2
1	A	45	GLN	2.2
1	A	71	GLN	2.2
8	H	88	SER	2.2
5	E	89	GLY	2.2
1	A	162	VAL	2.1
13	M	119	MET	2.1
1	A	153	PRO	2.1
5	E	119	SER	2.1
1	A	1288	ASP	2.1
9	I	81	ARG	2.1
2	B	87	LYS	2.1
13	M	117	ASN	2.1
5	E	82	PHE	2.0
2	B	440	HIS	2.0
13	M	88	ASP	2.0
13	M	201	LYS	2.0
13	M	206	THR	2.0
1	A	420	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
8	H	126	GLU	2.0
2	B	247	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
15	MG	A	2458	1/1	0.87	0.31	13.19	75,75,75,75	0
14	ZN	I	1121	1/1	0.99	0.08	-0.98	78,78,78,78	0
14	ZN	A	2457	1/1	0.99	0.12	-1.10	51,51,51,51	0
14	ZN	B	2225	1/1	1.00	0.14	-1.36	46,46,46,46	0
14	ZN	J	1066	1/1	1.00	0.15	-1.42	46,46,46,46	0
14	ZN	C	1269	1/1	0.99	0.07	-1.59	64,64,64,64	0
14	ZN	L	1071	1/1	0.98	0.06	-1.67	98,98,98,98	0
14	ZN	M	1216	1/1	0.99	0.07	-2.17	73,73,73,73	0
14	ZN	A	2456	1/1	0.99	0.06	-2.54	91,91,91,91	0
14	ZN	I	1122	1/1	0.98	0.03	-2.82	130,130,130,130	0
15	MG	A	2459	1/1	0.82	0.44	-	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.