Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 06:04 AM EDT

PDB ID	:	4GZZ
Title	:	Crystal structures of bacterial RNA Polymerase paused elongation complexes
Authors	:	Weixlbaumer, A.; Leon, K.; Landick, R.; Darst, S.A.
Deposited on	:	2012-09-06
Resolution	:	4.29 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 (i) 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 (1)) were used in the production of this report:

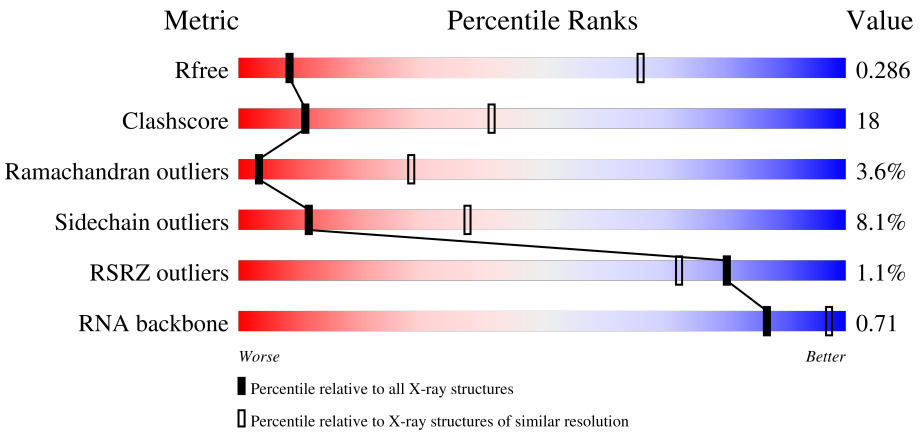
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 4.29 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)
RNA backbone	3102	1058 (5.60-3.00)

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 <=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	315	.% 42% 26% • 29%
1	B	315	48% 22% • 29%
2	C	1119	54% 38% 5% •
3	D	1534	2% 50% 34% 5% 11%

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Mol	Chain	Length	Quality of chain
4	E	99	% 40% 45% 7% 6%
5	N	13	46% 38% 15%
6	R	16	6% 44% 6% 44%
7	T	22	50% 50%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 24400 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
			Total	C	N	O	S			
1	A	223	1759	1123	306	328	2	0	0	0
1	B	223	1759	1123	306	328	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1083	8548	5412	1524	1588	24	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1358	10714	6780	1900	2001	33	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1525	HIS	-	expression tag	UNP Q8RQE8
D	1526	HIS	-	expression tag	UNP Q8RQE8
D	1527	HIS	-	expression tag	UNP Q8RQE8
D	1528	HIS	-	expression tag	UNP Q8RQE8
D	1529	HIS	-	expression tag	UNP Q8RQE8
D	1530	HIS	-	expression tag	UNP Q8RQE8
D	1531	HIS	-	expression tag	UNP Q8RQE8
D	1532	HIS	-	expression tag	UNP Q8RQE8
D	1533	HIS	-	expression tag	UNP Q8RQE8
D	1534	HIS	-	expression tag	UNP Q8RQE8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	93	754	481	131	138	4	0	0	0

- Molecule 5 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	N	11	225	107	43	64	11	0	0	0

- Molecule 6 is a RNA chain called RNA transcript.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	R	9	191	85	31	66	9	0	0	0

- Molecule 7 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	T	22	447	213	81	131	22	0	0	0

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

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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

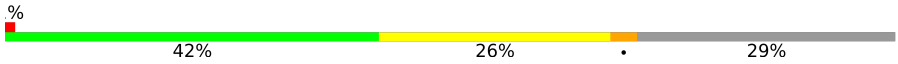
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
9	D	1	1	1	0	0

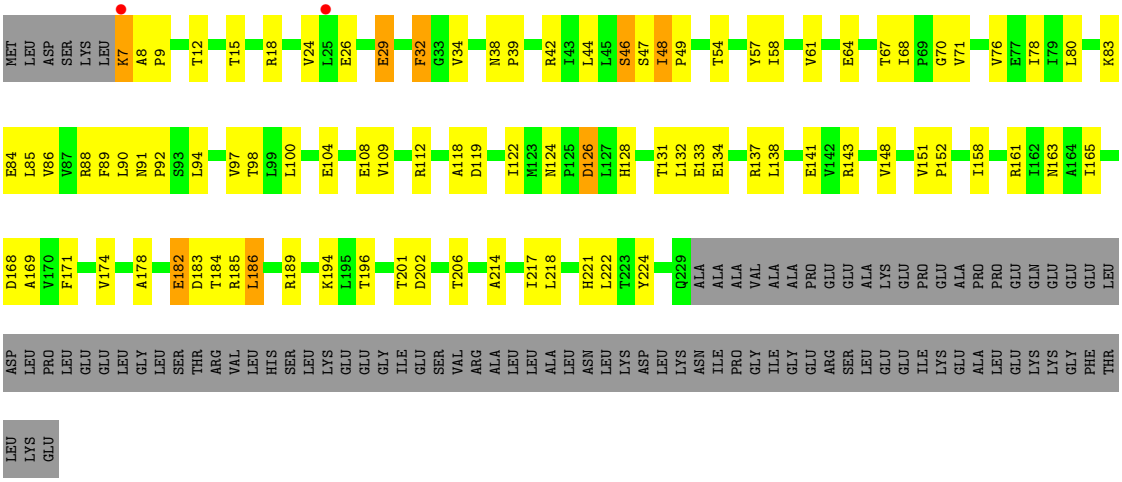
3 Residue-property plots (i)

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

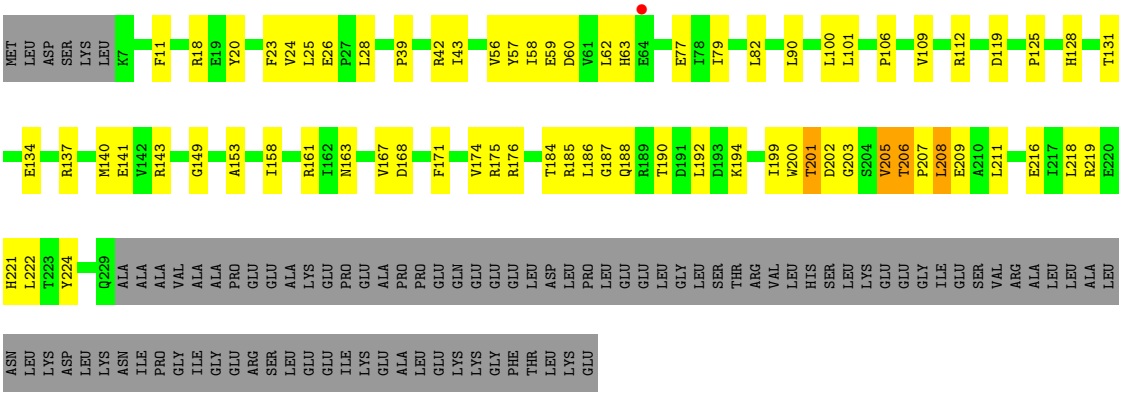
Chain A:





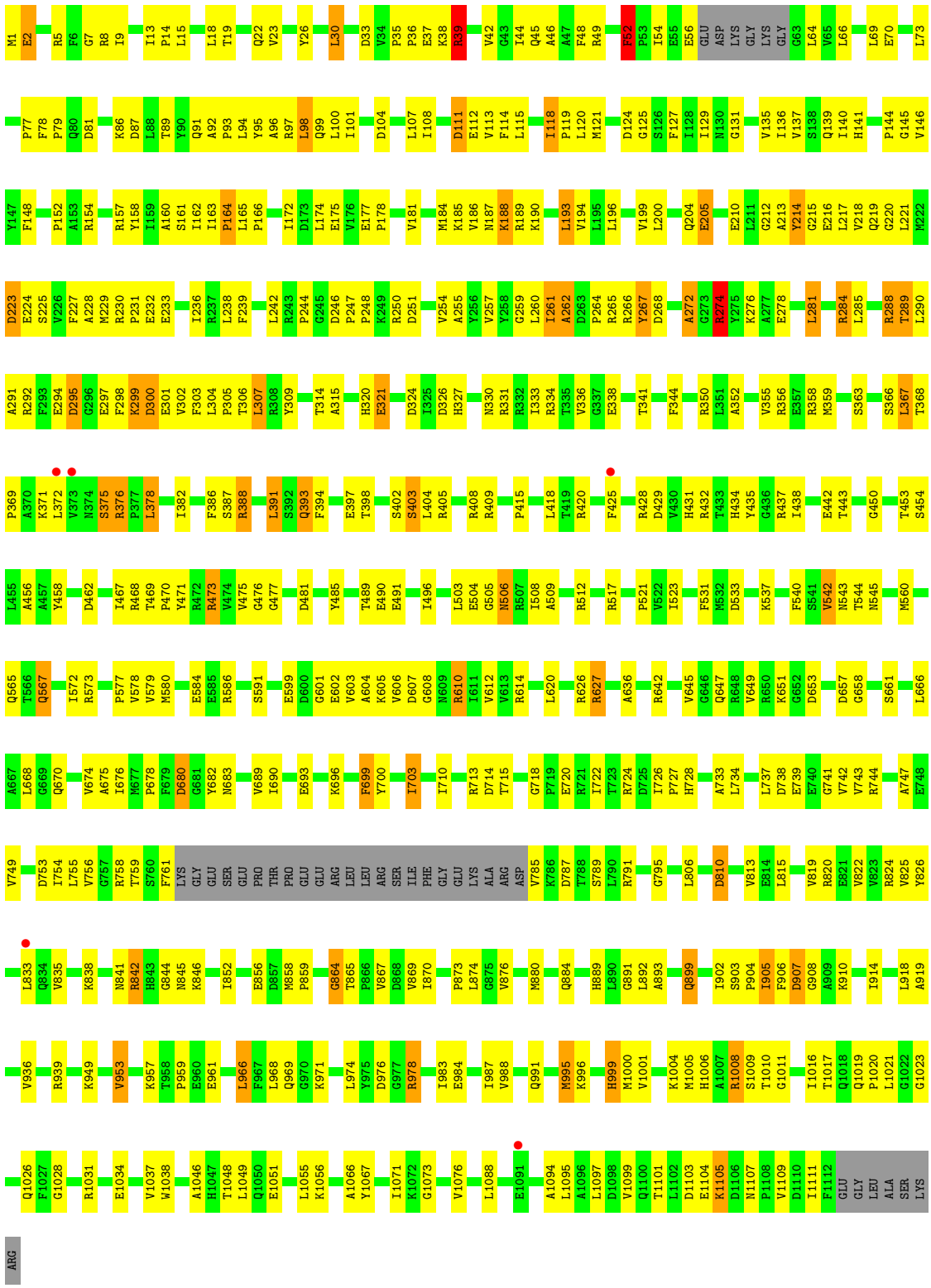
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



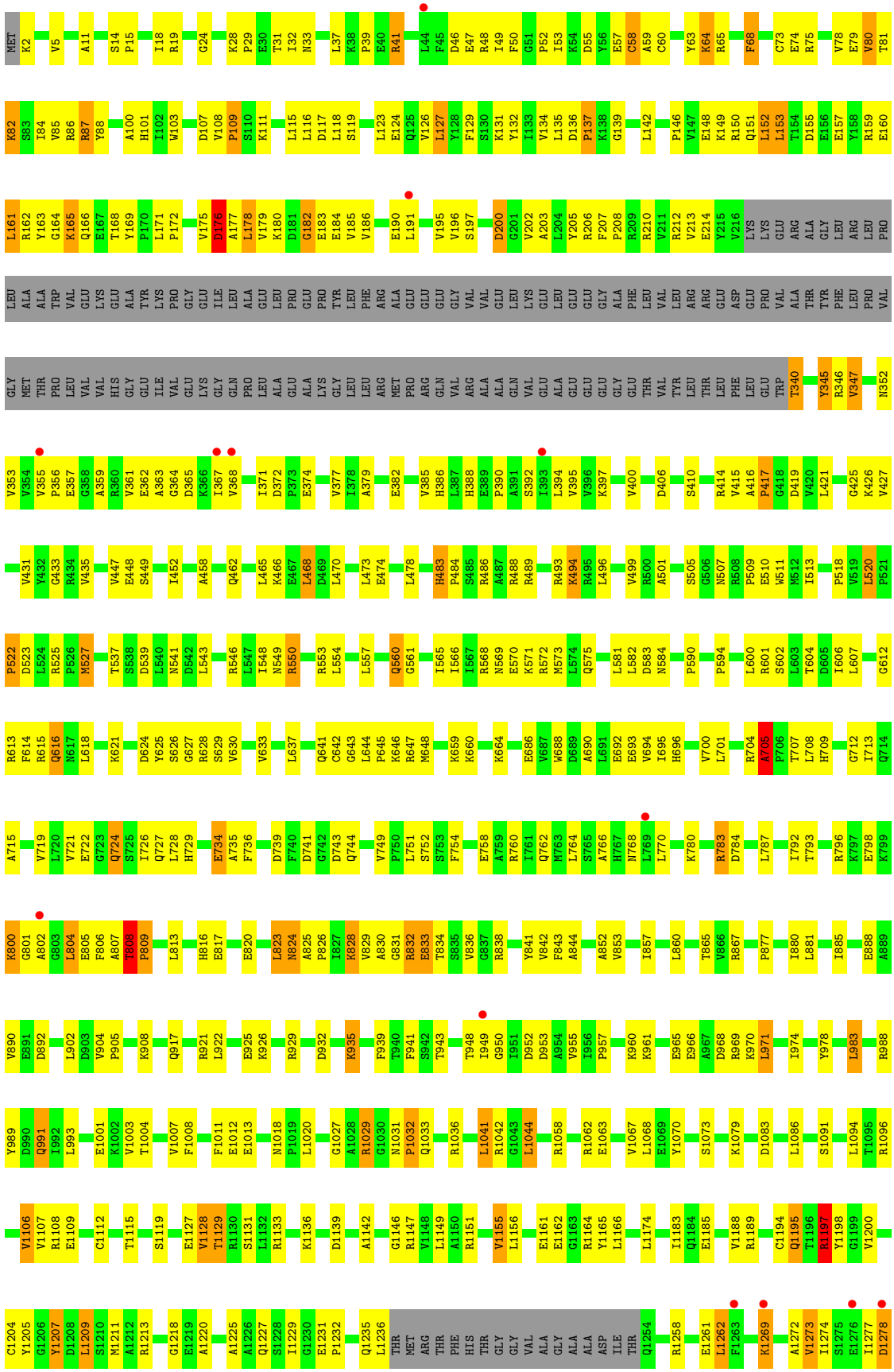
• Molecule 2: DNA-directed RNA polymerase subunit beta

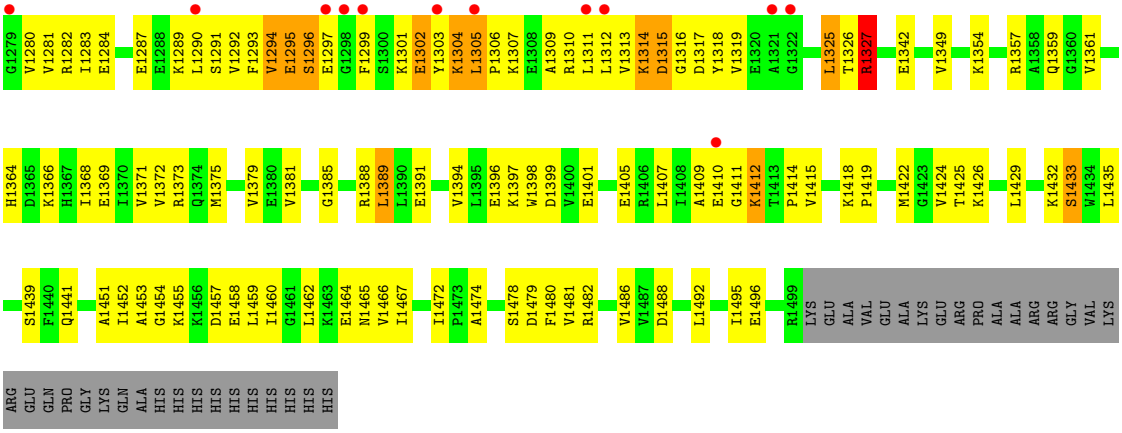
Chain C:



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

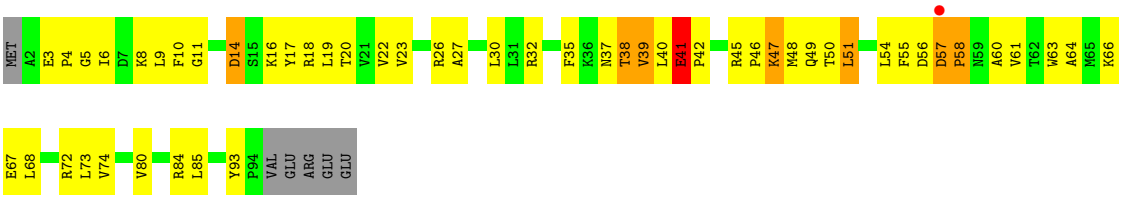
Chain D:


MET K2 V5 A11 S14 P15 I18 R19 G24 K28 P29 E30 T31 I32 N33 L37 K38 P39 E40 R41 L44 F45 D46 E47 R48 I49 F50 G51 P52 I53 K54 D55 Y56 E57 C58 A59 C60 Y63 K64 R65 F68 C73 E74 R75 V78 E79 V80 T81
K82 S83 I84 V85 R86 R87 Y88 A100 H101 I102 W103 D107 V108 P109 S110 K111 L115 L116 D117 L118 S119 L123 E124 Q125 V126 L127 Y128 F129 S130 K131 Y132 I133 V134 L135 D136 P137 K138 G139 L142 P146 V147 E148 K149 R150 Q151 L152 L153 T154 D155 E156 E157 Y158 R159 E160
L161 R162 Y163 G164 K165 Q166 E167 T168 Y169 P170 L171 P172 V175 D176 A177 L178 V179 K180 D181 G182 E183 E184 V185 V186 E190 L191 V195 V196 S197 D200 G201 V202 A203 L204 Y205 R206 F207 P208 R209 R210 V211 R212 V213 E214 Y215 V216 LYS LYS GLU ARG ALA GLY LEU ARG LEU PRO
LEU ALA ALA TRP VAL GLU LYS LYS GLU ALA TYR TYR LYS PRO GLY GLU ILE LEU ALA GLU LEU PRO GLU PRO TYR TYR LEU PHE ARG ALA GLU GLU GLU GLU GLY VAL VAL VAL GLU LEU LYS GLU LEU LEU GLU GLU GLY ALA PHE LEU VAL LEU ARG ARG GLU ASP GLU PRO VAL ALA THR TYR PHE LEU PRO VAL
GLY MET THR PRO LEU VAL VAL HIS GLY GLU ILE VAL GLU LYS GLY GLN PRO LEU ALA GLU ALA LYS LYS GLY LEU LEU ARG MET PRO ARG GLN VAL ARG ALA ALA GLN VAL GLU ALA GLU GLU GLU GLY GLU THR VAL TYR LEU THR LEU PHE LEU GLU TRP T340 Y345 R346 V347 N352
V353 V354 V355 P356 E357 G358 A359 R360 V361 E362 A363 G364 D365 K366 I367 V368 I371 D372 P373 E374 V377 I378 A379 E382 V385 H386 L387 H388 E389 P390 A391 S392 I393 L394 V395 V396 K397 V400 D406 S410 R414 V415 A416 P417 G418 D419 V420 L421 G425 K426 V427
V431 Y432 G433 R434 V435 V447 E448 S449 I452 A458 Q462 L465 K466 E467 L468 D469 L470 L473 E474 L478 H483 P484 S485 R486 A487 R488 R489 R493 K494 R495 L496 V499 R500 A501 S505 G506 N507 R508 P509 E510 W511 M512 I513 P518 V519 L520 P521
P522 D523 L524 R525 P526 M527 T537 S538 D539 L540 N541 D542 L543 R546 L547 I548 N549 R550 R553 L554 L557 Q560 G561 I565 I566 I567 R568 N569 E570 K571 R572 M573 L574 Q575 L581 L582 D583 N584 P590 P594 L600 R601 S602 L603 T604 D605 I606 L607 G612
R613 F614 R615 Q616 M617 L618 K621 D624 Y625 S626 G627 R628 S629 V630 V633 L637 Q641 C642 G643 L644 P645 K646 R647 M648 K659 K660 K664 E686 V687 W688 D689 A690 L691 E692 E693 V694 I695 H696 V700 L701 R704 A705 P706 T707 L708 H709 G712 I713 Q714
A715 V719 L720 V721 E722 G723 Q724 S725 I726 Q727 L728 H729 E734 A735 F736 D739 F740 D741 G742 D743 Q744 V749 P750 L751 S752 S753 F754 E758 A759 R760 I761 Q762 M763 L764 S765 A766 H767 N768 L769 L770 K780 R783 D784 L787 I792 T793 R796 K797 E798 K799
K800 G801 A802 G803 L804 E805 F806 A807 T808 P809 L813 H816 E817 E820 L823 N824 A825 P826 I827 K828 V829 A830 G831 R832 E833 T834 S835 V836 G837 R838 Y841 V842 F843 A844 A852 V853 I857 L860 T865 V866 R867 P877 I880 L881 I885 E888 A889
V890 E891 D892 L902 D903 V904 P905 K908 Q917 R921 L922 E925 K926 R929 D932 K935 F939 T940 F941 S942 T943 T948 I949 G950 I951 D952 D953 A954 V955 I956 P957 K960 K961 E965 E966 A967 D968 R969 K970 L971 I974 Y978 L983 R988
Y989 D990 Q991 I992 L993 E1001 K1002 V1003 T1004 V1007 F1008 F1011 E1012 E1013 N1018 P1019 L1020 G1027 A1028 R1029 G1030 N1031 P1032 Q1033 R1036 L1041 R1042 G1043 L1044 R1058 R1062 E1063 V1067 L1068 E1069 Y1070 S1073 K1079 D1083 L1086 S1091 L1094 T1095 R1096
V1106 V1107 R1108 E1109 C1112 T1115 S1119 E1127 V1128 T1129 R1130 S1131 L1132 R1133 K1136 D1139 A1142 G1146 R1147 V1148 L1149 A1150 R1151 V1155 L1156 E1161 E1162 G1163 R1164 Y1165 L1166 L1174 I1183 Q1184 E1185 V1188 R1189 C1194 Q1195 T1196 R1197 Y1198 G1199 V1200
C1204 Y1205 G1206 Y1207 D1208 L1209 S1210 M1211 A1212 R1213 G1218 E1219 A1220 A1225 A1226 Q1227 S1228 I1229 G1230 E1231 P1232 Q1235 L1236 THR MET ARG THR PHE HIS THR GLY GLY VAL ALA GLY ALA ALA ASP ILE THR Q1254 R1258 E1261 L1262 F1263 K1269 A1272 V1273 I1274 S1275 E1276 I1277 D1278



• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

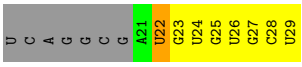


• Molecule 5: non-template DNA

Chain N:

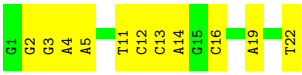
• Molecule 6: RNA transcript

Chain R:



• Molecule 7: template DNA

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	286.55Å 286.55Å 199.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.78 – 4.29 38.79 – 4.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.78-4.29) 87.8 (38.79-4.29)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 4.28Å)	Xtriage
Refinement program	PHENIX 1.8_1069, CNS	Depositor
R, R_{free}	0.234 , 0.285 0.236 , 0.286	Depositor DCC
R_{free} test set	2074 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	164.3	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	24400	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.26	0/1791	0.47	0/2436
1	B	0.28	0/1791	0.47	0/2436
2	C	0.28	0/8711	0.51	0/11784
3	D	0.28	0/10897	0.50	1/14726 (0.0%)
4	E	0.29	0/768	0.55	0/1035
5	N	0.44	0/252	1.08	0/386
6	R	0.21	0/212	0.77	0/328
7	T	0.44	0/500	1.08	0/768
All	All	0.29	0/24922	0.53	1/33899 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	705	ALA	C-N-CD	5.17	139.25	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1805	65	0
1	B	1759	0	1805	50	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8548	0	8650	371	0
3	D	10714	0	10936	408	1
4	E	754	0	769	40	0
5	N	225	0	124	3	0
6	R	191	0	95	10	0
7	T	447	0	248	10	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	24400	0	24432	882	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (882) 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)
2:C:428:ARG:HH12	3:D:1086:LEU:HD21	1.24	0.98
2:C:610:ARG:HG3	2:C:610:ARG:HH11	1.27	0.96
2:C:846:LYS:NZ	6:R:29:U:OP1	1.99	0.96
1:B:188:GLN:O	3:D:646:LYS:NZ	2.00	0.94
1:A:80:LEU:HD21	2:C:573:ARG:HH11	1.34	0.92
2:C:194:VAL:HG21	2:C:224:GLU:HG3	1.57	0.87
3:D:808:THR:H	3:D:809:PRO:HD2	1.37	0.86
3:D:925:GLU:O	3:D:929:ARG:NH1	2.08	0.86
2:C:274:ARG:NH1	2:C:284:ARG:HH12	1.72	0.86
2:C:388:ARG:NH1	7:T:22:DT:OP1	2.09	0.85
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.58	0.85
3:D:629:SER:HB3	3:D:726:ILE:HG12	1.61	0.81
3:D:1128:VAL:HG23	3:D:1133:ARG:HH22	1.43	0.81
1:A:34:VAL:HG21	2:C:939:ARG:HE	1.45	0.81
2:C:738:ASP:HB2	2:C:744:ARG:HB3	1.61	0.81
2:C:274:ARG:HH12	2:C:284:ARG:HH12	1.26	0.80
2:C:290:LEU:HD13	2:C:302:VAL:HG12	1.64	0.80
3:D:501:ALA:HB1	3:D:1453:ALA:HB2	1.64	0.80
2:C:224:GLU:HB3	2:C:227:PHE:HB3	1.62	0.80
1:A:151:VAL:HB	1:A:169:ALA:HB3	1.64	0.79
2:C:292:ARG:NH1	2:C:294:GLU:HB2	1.97	0.78
3:D:136:ASP:HB2	3:D:137:PRO:HD2	1.66	0.78
3:D:161:LEU:O	3:D:397:LYS:NZ	2.17	0.78
2:C:1008:ARG:HD2	2:C:1026:GLN:HB3	1.66	0.77
2:C:292:ARG:HH12	2:C:294:GLU:HB2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1106:VAL:HG12	3:D:1220:ALA:HA	1.63	0.77
3:D:213:VAL:HG11	3:D:385:VAL:HA	1.67	0.77
2:C:1008:ARG:HH12	2:C:1011:GLY:N	1.82	0.76
1:A:18:ARG:HG3	1:A:206:THR:HG22	1.67	0.76
1:A:108:GLU:HG2	1:A:131:THR:HG22	1.67	0.76
3:D:1209:LEU:HD11	4:E:16:LYS:HD2	1.67	0.76
1:A:182:GLU:HB2	1:A:194:LYS:HD3	1.69	0.75
2:C:1051:GLU:HG3	2:C:1055:LEU:HD23	1.67	0.75
2:C:584:GLU:HB3	2:C:666:LEU:H	1.52	0.75
2:C:720:GLU:O	2:C:820:ARG:NH2	2.20	0.74
2:C:52:PHE:HE1	2:C:98:LEU:HD13	1.53	0.74
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.70	0.74
2:C:437:ARG:HD3	2:C:467:ILE:HB	1.68	0.74
1:B:205:VAL:HG13	1:B:209:GLU:HB2	1.69	0.74
2:C:714:ASP:OD1	2:C:820:ARG:NH1	2.21	0.74
3:D:983:LEU:HD13	3:D:988:ARG:HB2	1.69	0.74
2:C:1103:ASP:HB3	2:C:1105:LYS:NZ	2.03	0.74
2:C:23:VAL:HA	2:C:121:MET:HE1	1.69	0.73
2:C:239:PHE:HB2	2:C:251:ASP:HB3	1.71	0.73
2:C:1105:LYS:HZ1	2:C:1107:ASN:HB2	1.54	0.73
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.71	0.73
2:C:610:ARG:HH11	2:C:610:ARG:CG	2.02	0.73
2:C:1105:LYS:NZ	2:C:1107:ASN:HB2	2.03	0.73
2:C:726:ILE:HD13	2:C:754:ILE:HD13	1.71	0.72
3:D:1165:TYR:HB3	3:D:1207:TYR:HE1	1.54	0.72
3:D:1283:ILE:HD11	3:D:1290:LEU:HD12	1.72	0.72
2:C:670:GLN:NE2	2:C:699:PHE:O	2.22	0.72
2:C:290:LEU:HD11	2:C:301:GLU:H	1.55	0.72
2:C:334:ARG:HH12	2:C:415:PRO:HG2	1.55	0.72
2:C:224:GLU:O	2:C:228:ALA:N	2.21	0.72
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.04	0.71
2:C:1048:THR:N	3:D:758:GLU:OE2	2.21	0.71
3:D:1194:CYS:SG	3:D:1195:GLN:N	2.63	0.71
3:D:127:LEU:HG	3:D:152:LEU:HD12	1.72	0.70
2:C:274:ARG:HH12	2:C:284:ARG:NH1	1.87	0.70
3:D:210:ARG:HB3	3:D:388:HIS:HB2	1.74	0.70
3:D:805:GLU:OE2	3:D:816:HIS:NE2	2.25	0.70
3:D:52:PRO:HG2	3:D:80:VAL:HG13	1.74	0.69
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.72	0.69
3:D:557:LEU:HD21	3:D:566:ILE:HG22	1.74	0.69
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:701:LEU:HB3	3:D:713:ILE:HD11	1.74	0.69
3:D:165:LYS:HE3	3:D:200:ASP:HB2	1.75	0.69
2:C:290:LEU:HD21	2:C:300:ASP:HB2	1.74	0.69
2:C:579:VAL:O	2:C:842:ARG:NH2	2.26	0.69
1:A:58:ILE:HB	1:A:61:VAL:HB	1.74	0.68
1:A:104:GLU:HB3	1:A:137:ARG:HG3	1.74	0.68
2:C:674:VAL:HG22	2:C:869:VAL:HB	1.75	0.68
3:D:798:GLU:HB2	3:D:828:LYS:HE3	1.76	0.68
3:D:852:ALA:HB1	3:D:857:ILE:HD11	1.74	0.68
2:C:260:LEU:HD22	2:C:288:ARG:HH22	1.58	0.68
3:D:346:ARG:NH1	3:D:347:VAL:O	2.27	0.68
4:E:46:PRO:HG3	4:E:66:LYS:HD3	1.76	0.68
2:C:22:GLN:NE2	2:C:136:ILE:O	2.25	0.68
2:C:976:ASP:OD1	2:C:978:ARG:NH1	2.26	0.68
3:D:169:TYR:HB3	3:D:195:VAL:HG11	1.75	0.68
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.75	0.68
2:C:734:LEU:HG	2:C:737:LEU:HD12	1.74	0.67
3:D:568:ARG:NH1	3:D:571:LYS:HE3	2.09	0.67
3:D:135:LEU:HD23	3:D:148:GLU:HB2	1.74	0.67
2:C:274:ARG:HH12	2:C:284:ARG:HH22	1.43	0.67
2:C:292:ARG:HB3	2:C:299:LYS:HZ2	1.59	0.67
3:D:820:GLU:HB2	3:D:836:VAL:HG21	1.76	0.67
1:B:90:LEU:HB2	1:B:119:ASP:HB3	1.76	0.66
2:C:1103:ASP:HB3	2:C:1105:LYS:HZ1	1.58	0.66
2:C:845:ASN:HB2	2:C:884:GLN:NE2	2.11	0.66
2:C:292:ARG:HG3	2:C:292:ARG:HH11	1.58	0.66
3:D:1495:ILE:HG23	4:E:84:ARG:HD3	1.75	0.66
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.76	0.66
1:B:59:GLU:HB3	1:B:137:ARG:HH12	1.61	0.66
3:D:493:ARG:NH2	3:D:1389:LEU:O	2.27	0.66
2:C:30:LEU:HB3	2:C:44:ILE:HD12	1.78	0.66
2:C:115:LEU:HA	2:C:375:SER:HB2	1.78	0.65
2:C:101:ILE:HD12	2:C:107:LEU:HD22	1.78	0.65
2:C:265:ARG:HH11	2:C:267:TYR:HD1	1.45	0.65
2:C:185:LYS:HG2	2:C:190:LYS:HG2	1.79	0.65
2:C:787:ASP:OD1	2:C:791:ARG:NH2	2.29	0.65
3:D:568:ARG:HH11	3:D:571:LYS:HE3	1.61	0.65
1:B:175:ARG:N	1:B:200:TRP:O	2.29	0.65
2:C:184:MET:HE2	2:C:193:LEU:HD12	1.79	0.65
2:C:824:ARG:NH2	2:C:826:TYR:OH	2.29	0.65
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:645:PRO:HG2	3:D:648:MET:HG3	1.78	0.65
3:D:1147:ARG:HD3	3:D:1188:VAL:HG21	1.78	0.65
3:D:770:LEU:HD12	3:D:1211:MET:HA	1.80	0.64
3:D:1273:VAL:HG12	3:D:1274:ILE:H	1.62	0.64
3:D:1147:ARG:HE	3:D:1364:HIS:HE1	1.44	0.64
2:C:428:ARG:NH1	3:D:1086:LEU:HD21	2.06	0.64
3:D:783:ARG:HH11	3:D:783:ARG:HG2	1.62	0.64
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.79	0.64
3:D:1273:VAL:HG21	3:D:1305:LEU:HD12	1.79	0.64
2:C:95:TYR:HD1	2:C:112:GLU:HB3	1.61	0.64
2:C:690:ILE:HG23	2:C:852:ILE:HG23	1.79	0.64
3:D:988:ARG:HA	3:D:991:GLN:HB2	1.79	0.64
6:R:24:U:O4	7:T:19:DA:N1	2.31	0.64
2:C:668:LEU:O	2:C:995:MET:HB3	1.97	0.63
3:D:362:GLU:O	3:D:364:GLY:N	2.22	0.63
3:D:414:ARG:HG3	3:D:433:GLY:H	1.63	0.63
3:D:950:GLY:N	3:D:953:ASP:OD2	2.30	0.63
3:D:1213:ARG:HH22	4:E:11:GLY:HA2	1.63	0.63
4:E:48:MET:HB2	4:E:54:LEU:HB2	1.81	0.63
6:R:24:U:H3	7:T:19:DA:H2	1.45	0.63
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.79	0.63
3:D:129:PHE:HB3	3:D:572:ARG:HG3	1.81	0.63
3:D:700:VAL:HG12	3:D:749:VAL:HG12	1.81	0.63
2:C:86:LYS:HD3	2:C:813:VAL:HG12	1.81	0.62
2:C:1009:SER:HA	3:D:625:TYR:HA	1.81	0.62
1:A:71:VAL:HG11	1:A:78:ILE:HD11	1.81	0.62
2:C:144:PRO:HB3	2:C:164:PRO:HA	1.82	0.62
2:C:264:PRO:HB2	2:C:289:THR:HG21	1.79	0.62
2:C:658:GLY:N	2:C:661:SER:OG	2.32	0.62
2:C:580:MET:HB2	2:C:584:GLU:OE2	1.99	0.62
3:D:163:TYR:O	3:D:165:LYS:N	2.29	0.62
1:B:62:LEU:HD23	1:B:163:ASN:HD22	1.65	0.62
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.81	0.62
3:D:1314:LYS:NZ	3:D:1316:GLY:HA3	2.14	0.62
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.81	0.62
2:C:309:TYR:CZ	2:C:321:GLU:HB3	2.35	0.62
3:D:501:ALA:O	3:D:505:SER:OG	2.15	0.61
3:D:1354:LYS:HA	3:D:1357:ARG:HD2	1.81	0.61
3:D:115:LEU:HD21	3:D:468:LEU:HD22	1.81	0.61
3:D:1294:VAL:HG11	3:D:1319:VAL:HG11	1.82	0.61
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:ARG:HH12	2:C:284:ARG:NH2	1.98	0.61
2:C:505:GLY:O	2:C:506:ASN:ND2	2.31	0.61
3:D:1232:PRO:HB2	3:D:1361:VAL:HG11	1.81	0.61
2:C:873:PRO:HB3	3:D:949:ILE:HG12	1.81	0.61
2:C:165:LEU:HG	2:C:166:PRO:HA	1.82	0.61
2:C:599:GLU:OE2	2:C:651:LYS:HD2	2.01	0.61
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.81	0.61
2:C:267:TYR:HB2	2:C:272:ALA:HB3	1.82	0.60
3:D:1405:GLU:HA	3:D:1409:ALA:HB3	1.81	0.60
1:A:112:ARG:NH2	1:A:126:ASP:OD1	2.35	0.60
2:C:578:VAL:HG13	2:C:579:VAL:HG23	1.83	0.60
2:C:607:ASP:OD1	2:C:608:GLY:N	2.34	0.60
3:D:87:ARG:HD2	3:D:88:TYR:CE1	2.37	0.60
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.84	0.60
2:C:259:GLY:HA2	2:C:291:ALA:HB2	1.83	0.60
3:D:917:GLN:HB3	3:D:921:ARG:NH1	2.17	0.60
3:D:473:LEU:HD23	3:D:499:VAL:HG21	1.84	0.60
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.83	0.60
2:C:7:GLY:HA3	2:C:904:PRO:HG2	1.83	0.60
2:C:184:MET:HB2	2:C:193:LEU:HB2	1.84	0.60
2:C:230:ARG:HB3	2:C:233:GLU:HB2	1.84	0.60
3:D:1394:VAL:HG21	3:D:1432:LYS:HZ1	1.66	0.60
2:C:759:THR:HG22	2:C:787:ASP:HA	1.84	0.60
3:D:184:GLU:HA	3:D:202:VAL:HA	1.82	0.60
3:D:1479:ASP:OD2	3:D:1482:ARG:NH2	2.34	0.60
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.83	0.60
2:C:978:ARG:CG	2:C:978:ARG:HH11	2.15	0.59
3:D:612:GLY:O	3:D:616:GLN:NE2	2.35	0.59
2:C:437:ARG:NH1	2:C:491:GLU:OE1	2.26	0.59
3:D:165:LYS:O	3:D:395:VAL:HG23	2.02	0.59
3:D:760:ARG:HD3	4:E:61:VAL:HG11	1.83	0.59
4:E:39:VAL:O	4:E:72:ARG:NH1	2.35	0.59
2:C:265:ARG:NH1	2:C:267:TYR:HD1	2.00	0.59
1:B:149:GLY:H	1:B:171:PHE:HB2	1.66	0.59
3:D:1174:LEU:HD22	3:D:1183:ILE:HD11	1.85	0.59
2:C:165:LEU:HD21	2:C:418:LEU:HD11	1.85	0.59
3:D:565:ILE:HD12	3:D:565:ILE:H	1.66	0.59
2:C:408:ARG:NH2	2:C:456:ALA:O	2.36	0.59
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.85	0.58
3:D:614:PHE:HB3	3:D:1439:SER:HA	1.85	0.58
3:D:618:LEU:HD11	3:D:1467:ILE:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:LYS:HZ2	2:C:299:LYS:HB3	1.67	0.58
1:A:80:LEU:HD21	2:C:573:ARG:NH1	2.12	0.58
2:C:1008:ARG:HH12	2:C:1010:THR:C	2.06	0.58
2:C:443:THR:HG22	2:C:453:THR:HG22	1.85	0.58
3:D:647:ARG:NH1	3:D:724:GLN:OE1	2.36	0.58
2:C:604:ALA:HB3	2:C:612:VAL:HB	1.85	0.58
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.84	0.58
2:C:223:ASP:OD1	2:C:224:GLU:HG2	2.04	0.58
2:C:755:LEU:HD11	2:C:825:VAL:HG11	1.85	0.58
3:D:1161:GLU:HB2	3:D:1164:ARG:HB2	1.85	0.58
2:C:38:LYS:HD2	2:C:39:ARG:NH1	2.18	0.58
2:C:216:GLU:O	2:C:218:VAL:N	2.37	0.58
1:B:206:THR:HG22	1:B:207:PRO:HD2	1.84	0.58
3:D:58:CYS:SG	3:D:59:ALA:N	2.77	0.58
3:D:660:LYS:HG3	3:D:694:VAL:HG12	1.86	0.58
4:E:14:ASP:OD1	4:E:14:ASP:N	2.30	0.58
3:D:1031:ASN:OD1	3:D:1033:GLN:NE2	2.36	0.57
2:C:18:LEU:HD21	2:C:542:VAL:HG11	1.86	0.57
2:C:537:LYS:HG2	2:C:905:ILE:HG12	1.86	0.57
3:D:520:LEU:HB3	3:D:525:ARG:HD3	1.85	0.57
2:C:473:ARG:HA	2:C:531:PHE:HA	1.85	0.57
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.86	0.57
2:C:52:PHE:CE1	2:C:98:LEU:HD13	2.36	0.57
3:D:368:VAL:HB	3:D:377:VAL:HG12	1.86	0.57
3:D:783:ARG:HG2	3:D:783:ARG:NH1	2.20	0.57
1:A:9:PRO:HG2	1:B:224:TYR:CE2	2.40	0.57
3:D:1480:PHE:O	4:E:18:ARG:NH1	2.38	0.57
1:A:85:LEU:HA	1:A:124:ASN:HD22	1.70	0.57
2:C:841:ASN:OD1	2:C:844:GLY:N	2.35	0.57
1:A:18:ARG:HH21	1:A:88:ARG:HD2	1.70	0.57
1:A:104:GLU:OE1	1:A:137:ARG:NH1	2.37	0.57
2:C:710:ILE:HD11	2:C:758:ARG:HH21	1.69	0.57
2:C:429:ASP:OD2	3:D:1079:LYS:HD3	2.05	0.56
3:D:1394:VAL:HB	3:D:1397:LYS:HG2	1.87	0.56
3:D:1418:LYS:HD3	3:D:1419:PRO:HD2	1.86	0.56
3:D:1458:GLU:O	3:D:1460:ILE:N	2.37	0.56
1:A:143:ARG:HH12	1:A:158:ILE:HD12	1.69	0.56
2:C:274:ARG:NH1	2:C:284:ARG:NH1	2.47	0.56
3:D:783:ARG:HD3	3:D:1029:ARG:HG2	1.86	0.56
1:B:174:VAL:HA	1:B:201:THR:HA	1.86	0.56
2:C:601:GLY:HA3	2:C:614:ARG:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:LEU:HD12	2:C:98:LEU:HD11	1.87	0.56
2:C:204:GLN:NE2	2:C:228:ALA:O	2.38	0.56
2:C:292:ARG:HB3	2:C:299:LYS:HB3	1.87	0.56
2:C:689:VAL:HB	2:C:870:ILE:HB	1.86	0.56
2:C:845:ASN:HB2	2:C:884:GLN:HE22	1.71	0.56
3:D:172:PRO:HG2	3:D:175:VAL:HG21	1.87	0.56
3:D:1131:SER:HB2	3:D:1133:ARG:NH2	2.21	0.56
2:C:858:MET:HG3	2:C:859:PRO:HD2	1.87	0.56
3:D:180:LYS:NZ	3:D:388:HIS:HE1	2.03	0.56
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.36	0.56
2:C:324:ASP:O	2:C:330:ASN:ND2	2.39	0.56
2:C:437:ARG:HG3	2:C:437:ARG:HH11	1.70	0.56
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.88	0.56
2:C:756:VAL:O	2:C:789:SER:HB3	2.06	0.56
3:D:179:VAL:HG13	3:D:183:GLU:HB3	1.87	0.56
2:C:437:ARG:HG2	2:C:469:THR:HG23	1.87	0.56
3:D:180:LYS:HZ1	3:D:388:HIS:HE1	1.54	0.56
3:D:210:ARG:HH21	3:D:346:ARG:HD3	1.71	0.56
1:A:132:LEU:HD21	1:A:138:LEU:HD23	1.88	0.55
2:C:145:GLY:H	2:C:163:ILE:HG23	1.71	0.55
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.42	0.55
2:C:91:GLN:HA	2:C:119:PRO:HA	1.88	0.55
4:E:72:ARG:HB2	4:E:73:LEU:HD12	1.88	0.55
3:D:345:TYR:CZ	3:D:377:VAL:HB	2.41	0.55
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.72	0.55
2:C:5:ARG:HG2	2:C:902:ILE:HB	1.89	0.55
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.40	0.55
1:A:7:LYS:HD3	1:A:186:LEU:HD22	1.88	0.55
1:A:143:ARG:NH1	1:A:158:ILE:HD12	2.22	0.55
2:C:326:ASP:HB2	2:C:331:ARG:NH1	2.22	0.55
3:D:1236:LEU:HD23	3:D:1359:GLN:HG3	1.88	0.55
2:C:200:LEU:HD22	2:C:300:ASP:HB3	1.89	0.55
3:D:182:GLY:HA2	3:D:203:ALA:O	2.07	0.55
3:D:800:LYS:NZ	3:D:804:LEU:HD13	2.22	0.55
2:C:194:VAL:HG12	2:C:221:LEU:HB2	1.89	0.55
1:A:29:GLU:OE2	1:A:189:ARG:HD2	2.07	0.54
1:B:185:ARG:NH2	3:D:688:TRP:HB3	2.23	0.54
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.89	0.54
2:C:739:GLU:HB2	2:C:742:VAL:HB	1.89	0.54
3:D:165:LYS:HD2	3:D:397:LYS:HG3	1.89	0.54
3:D:801:GLY:HA3	3:D:825:ALA:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1107:VAL:O	3:D:1218:GLY:N	2.37	0.54
3:D:1128:VAL:HG23	3:D:1133:ARG:NH2	2.18	0.54
3:D:494:LYS:HB2	3:D:494:LYS:NZ	2.23	0.54
3:D:1425:THR:O	3:D:1429:LEU:HB2	2.08	0.54
2:C:46:ALA:HB1	2:C:266:ARG:NH1	2.23	0.54
2:C:292:ARG:NH1	2:C:292:ARG:HG3	2.23	0.54
3:D:484:PRO:HB3	3:D:488:ARG:NE	2.22	0.54
3:D:486:ARG:HE	3:D:489:ARG:HD2	1.71	0.54
3:D:764:LEU:HD23	3:D:766:ALA:H	1.71	0.54
1:B:216:GLU:OE2	1:B:219:ARG:NH2	2.41	0.54
2:C:54:ILE:HG22	2:C:66:LEU:HD23	1.89	0.54
2:C:398:THR:HG21	2:C:567:GLN:HA	1.89	0.54
2:C:140:ILE:HG12	2:C:333:ILE:HG12	1.90	0.54
3:D:139:GLY:HA2	3:D:452:ILE:HG12	1.90	0.54
3:D:421:LEU:HB2	3:D:427:VAL:HG12	1.88	0.54
3:D:607:LEU:HD23	3:D:614:PHE:HE1	1.73	0.54
3:D:1277:ILE:HG13	3:D:1301:LYS:NZ	2.23	0.54
3:D:784:ASP:HB3	3:D:939:PHE:CE1	2.42	0.54
3:D:842:VAL:HG12	3:D:865:THR:HB	1.90	0.54
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.90	0.54
1:A:174:VAL:HA	1:A:201:THR:HG22	1.89	0.54
2:C:97:ARG:HG2	2:C:111:ASP:HB3	1.89	0.54
3:D:800:LYS:HZ2	3:D:804:LEU:HD13	1.72	0.54
2:C:18:LEU:HD22	2:C:404:LEU:HD21	1.89	0.53
2:C:233:GLU:N	2:C:233:GLU:OE1	2.41	0.53
3:D:165:LYS:HB2	3:D:397:LYS:HB2	1.90	0.53
2:C:146:VAL:HB	2:C:281:LEU:HD11	1.89	0.53
3:D:31:THR:OG1	3:D:32:ILE:N	2.39	0.53
2:C:1038:TRP:HB3	3:D:1227:GLN:HE21	1.73	0.53
2:C:274:ARG:HH12	2:C:284:ARG:CZ	2.21	0.53
2:C:580:MET:O	2:C:903:SER:N	2.35	0.53
3:D:361:VAL:HG13	3:D:365:ASP:HB2	1.91	0.53
3:D:626:SER:OG	3:D:627:GLY:N	2.42	0.53
2:C:274:ARG:HH21	2:C:278:GLU:HB2	1.73	0.53
3:D:1396:GLU:HA	3:D:1399:ASP:OD2	2.08	0.53
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.91	0.53
2:C:158:TYR:HD1	2:C:314:THR:HG22	1.73	0.53
3:D:1281:VAL:O	3:D:1315:ASP:HA	2.09	0.53
2:C:987:ILE:HA	3:D:948:THR:HG21	1.90	0.53
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.73	0.53
3:D:1281:VAL:HG11	3:D:1313:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:LEU:HD13	2:C:261:ILE:HG13	1.91	0.53
1:A:85:LEU:HD12	1:A:124:ASN:HB3	1.90	0.52
2:C:255:ALA:HB1	2:C:298:PHE:CE1	2.44	0.52
3:D:153:LEU:HD23	3:D:153:LEU:H	1.73	0.52
3:D:155:ASP:O	3:D:159:ARG:HG2	2.09	0.52
3:D:367:ILE:HG13	3:D:377:VAL:HG13	1.90	0.52
2:C:375:SER:O	2:C:375:SER:OG	2.24	0.52
2:C:713:ARG:HA	2:C:819:VAL:HA	1.90	0.52
3:D:664:LYS:NZ	3:D:693:GLU:OE2	2.41	0.52
1:B:163:ASN:OD1	1:B:163:ASN:N	2.43	0.52
2:C:48:PHE:O	2:C:52:PHE:HB2	2.10	0.52
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.39	0.52
3:D:1258:ARG:NH1	3:D:1262:LEU:HD11	2.24	0.52
2:C:44:ILE:HG23	2:C:344:PHE:CE2	2.45	0.52
2:C:404:LEU:HD22	2:C:591:SER:HB3	1.90	0.52
3:D:832:ARG:NE	3:D:833:GLU:OE2	2.42	0.52
4:E:54:LEU:HD23	4:E:58:PRO:HD2	1.89	0.52
2:C:489:THR:HG23	2:C:490:GLU:HG3	1.92	0.52
4:E:17:TYR:O	4:E:20:THR:OG1	2.21	0.52
2:C:602:GLU:H	2:C:614:ARG:HB3	1.74	0.52
1:B:25:LEU:HD23	1:B:28:LEU:HD21	1.92	0.52
1:B:106:PRO:HG3	1:B:134:GLU:OE2	2.08	0.52
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.92	0.52
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.91	0.52
2:C:806:LEU:HB2	2:C:822:VAL:HG22	1.91	0.52
3:D:397:LYS:HD3	3:D:448:GLU:HB3	1.90	0.52
1:A:133:GLU:HG2	1:A:134:GLU:H	1.74	0.52
2:C:144:PRO:HA	2:C:163:ILE:HG23	1.90	0.52
3:D:637:LEU:HB2	3:D:641:GLN:HG3	1.92	0.52
3:D:1155:VAL:HG23	3:D:1156:LEU:H	1.73	0.52
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.92	0.52
2:C:504:GLU:HG3	2:C:509:ALA:HB2	1.91	0.52
2:C:236:ILE:HA	2:C:251:ASP:OD2	2.10	0.51
3:D:127:LEU:HD23	3:D:134:VAL:HB	1.91	0.51
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.39	0.51
3:D:19:ARG:NH1	3:D:19:ARG:HB2	2.25	0.51
3:D:925:GLU:OE1	4:E:6:ILE:N	2.44	0.51
2:C:1088:LEU:HD13	3:D:613:ARG:HG3	1.92	0.51
3:D:87:ARG:HB2	3:D:523:ASP:HB3	1.93	0.51
3:D:111:LYS:HD2	3:D:1452:ILE:HD13	1.93	0.51
1:B:58:ILE:HG23	1:B:140:MET:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:ASP:OD2	2:C:125:GLY:N	2.44	0.51
2:C:186:VAL:O	2:C:188:LYS:N	2.43	0.51
2:C:338:GLU:HA	2:C:341:THR:HG22	1.93	0.51
2:C:540:PHE:HB3	2:C:544:THR:HB	1.92	0.51
4:E:54:LEU:HA	4:E:58:PRO:HG2	1.93	0.51
2:C:1009:SER:HB2	3:D:625:TYR:CD1	2.45	0.51
3:D:525:ARG:NH1	3:D:541:ASN:OD1	2.44	0.51
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.75	0.51
3:D:957:PRO:HG3	3:D:1007:VAL:HA	1.93	0.51
1:A:44:LEU:HD23	1:A:48:ILE:HD11	1.91	0.51
1:A:98:THR:HG22	1:A:143:ARG:HG3	1.92	0.51
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.31	0.51
2:C:35:PRO:HD2	2:C:38:LYS:HG3	1.93	0.51
2:C:37:GLU:OE2	2:C:38:LYS:HG2	2.10	0.51
2:C:442:GLU:HG2	2:C:454:SER:HB2	1.92	0.51
2:C:18:LEU:HB3	2:C:404:LEU:HD11	1.93	0.51
2:C:48:PHE:HB3	2:C:52:PHE:HD2	1.76	0.51
2:C:978:ARG:HH11	2:C:978:ARG:HG2	1.76	0.51
3:D:458:ALA:HB2	3:D:575:GLN:HE22	1.76	0.51
3:D:616:GLN:HG3	3:D:621:LYS:NZ	2.26	0.51
4:E:26:ARG:HH21	4:E:30:LEU:HD13	1.76	0.51
2:C:141:HIS:HB2	2:C:418:LEU:HD22	1.92	0.51
2:C:284:ARG:NH1	2:C:285:LEU:H	2.09	0.51
2:C:1095:LEU:HD23	3:D:101:HIS:HE2	1.74	0.51
2:C:46:ALA:HB1	2:C:266:ARG:HH12	1.76	0.50
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.93	0.50
2:C:141:HIS:HE1	2:C:334:ARG:HG3	1.76	0.50
2:C:259:GLY:CA	2:C:291:ALA:HB2	2.41	0.50
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.47	0.50
2:C:458:TYR:HB3	2:C:470:PRO:HG3	1.93	0.50
2:C:610:ARG:HG3	2:C:610:ARG:NH1	2.08	0.50
3:D:415:VAL:HG21	3:D:421:LEU:HD21	1.92	0.50
3:D:695:ILE:HG13	3:D:696:HIS:H	1.76	0.50
3:D:728:LEU:HD21	3:D:736:PHE:HZ	1.75	0.50
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.46	0.50
2:C:38:LYS:NZ	2:C:38:LYS:HB3	2.27	0.50
2:C:521:PRO:HG3	3:D:1068:LEU:HD21	1.94	0.50
2:C:606:VAL:H	2:C:645:VAL:HG22	1.76	0.50
2:C:680:ASP:H	3:D:943:THR:HG21	1.76	0.50
2:C:1004:LYS:HD3	3:D:744:GLN:OE1	2.12	0.50
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:89:THR:HG22	2:C:129:ILE:HA	1.92	0.50
2:C:139:GLN:OE1	2:C:334:ARG:NH1	2.45	0.50
3:D:103:TRP:NE1	3:D:604:THR:OG1	2.41	0.50
1:B:176:ARG:NH2	3:D:888:GLU:OE2	2.45	0.50
2:C:1:MET:O	2:C:899:GLN:HA	2.12	0.50
2:C:636:ALA:HB3	2:C:703:ILE:HG13	1.93	0.50
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.93	0.50
3:D:690:ALA:O	3:D:694:VAL:HG13	2.12	0.50
3:D:1278:ASP:OD2	3:D:1278:ASP:N	2.40	0.50
3:D:1453:ALA:O	3:D:1455:LYS:N	2.44	0.50
1:B:184:THR:O	1:B:192:LEU:HB2	2.11	0.49
2:C:718:GLY:HA3	2:C:761:PHE:CD2	2.47	0.49
3:D:1213:ARG:NH2	4:E:10:PHE:O	2.45	0.49
1:A:38:ASN:O	1:A:42:ARG:HG2	2.12	0.49
2:C:649:VAL:HG12	2:C:653:ASP:HB3	1.94	0.49
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	1.93	0.49
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.94	0.49
2:C:363:SER:H	2:C:371:LYS:HE3	1.77	0.49
3:D:101:HIS:ND1	3:D:582:LEU:HD13	2.27	0.49
3:D:758:GLU:O	3:D:762:GLN:HG2	2.12	0.49
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.92	0.49
2:C:175:GLU:OE1	2:C:190:LYS:NZ	2.41	0.49
2:C:733:ALA:HB1	2:C:754:ILE:HD12	1.93	0.49
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.12	0.49
3:D:191:LEU:HG	3:D:197:SER:HB2	1.94	0.49
3:D:628:ARG:HH12	7:T:16:DC:H2"	1.76	0.49
2:C:893:ALA:HB2	2:C:918:LEU:HD23	1.94	0.49
3:D:646:LYS:HB3	3:D:688:TRP:CH2	2.47	0.49
1:B:24:VAL:HG11	1:B:194:LYS:NZ	2.27	0.49
2:C:919:ALA:HB2	2:C:968:LEU:HD21	1.94	0.49
3:D:126:VAL:HG13	3:D:132:TYR:HD2	1.78	0.49
3:D:1008:PHE:HZ	3:D:1032:PRO:HA	1.78	0.49
2:C:292:ARG:CB	2:C:299:LYS:HZ2	2.25	0.49
2:C:1006:HIS:HB2	3:D:628:ARG:HG2	1.94	0.49
3:D:116:LEU:O	3:D:118:LEU:HG	2.12	0.49
4:E:5:GLY:HA3	4:E:8:LYS:HE3	1.93	0.49
2:C:443:THR:CG2	2:C:453:THR:HG22	2.43	0.49
3:D:365:ASP:O	3:D:379:ALA:HB2	2.13	0.49
3:D:505:SER:OG	3:D:1453:ALA:HA	2.13	0.49
2:C:113:VAL:O	2:C:115:LEU:N	2.43	0.49
1:B:60:ASP:OD1	1:B:60:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1103:ASP:OD2	2:C:1104:GLU:N	2.40	0.48
3:D:802:ALA:HB3	3:D:824:ASN:HB3	1.95	0.48
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.94	0.48
2:C:876:VAL:HG11	3:D:949:ILE:HG21	1.95	0.48
2:C:999:HIS:CE1	6:R:28:C:H4'	2.47	0.48
3:D:50:PHE:CD1	3:D:522:PRO:HD3	2.48	0.48
3:D:152:LEU:CD2	3:D:152:LEU:H	2.26	0.48
2:C:69:LEU:HD13	2:C:99:GLN:HG2	1.95	0.48
4:E:47:LYS:HB3	4:E:55:PHE:CE2	2.48	0.48
6:R:22:U:H2'	6:R:23:G:C8	2.48	0.48
2:C:292:ARG:NH2	2:C:294:GLU:OE1	2.46	0.48
3:D:615:ARG:NE	3:D:1439:SER:O	2.41	0.48
3:D:1041:LEU:H	3:D:1041:LEU:HD22	1.77	0.48
1:A:7:LYS:NZ	1:A:7:LYS:HB3	2.28	0.48
2:C:726:ILE:HD11	2:C:754:ILE:HG21	1.94	0.48
2:C:1005:MET:HB2	3:D:724:GLN:HE22	1.78	0.48
3:D:136:ASP:CB	3:D:137:PRO:HD2	2.40	0.48
3:D:1457:ASP:OD2	3:D:1464:GLU:OE2	2.31	0.48
3:D:1495:ILE:HD12	4:E:84:ARG:HG2	1.94	0.48
2:C:185:LYS:HD2	2:C:190:LYS:HE2	1.95	0.48
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.96	0.48
3:D:719:VAL:O	3:D:721:VAL:HG23	2.14	0.48
3:D:784:ASP:HB3	3:D:939:PHE:HE1	1.78	0.48
3:D:152:LEU:H	3:D:152:LEU:HD23	1.78	0.48
3:D:970:LYS:HE3	3:D:974:ILE:HD11	1.96	0.48
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.78	0.48
3:D:207:PHE:O	3:D:390:PRO:HA	2.14	0.48
3:D:546:ARG:HA	3:D:549:ASN:HB2	1.96	0.48
3:D:704:ARG:NH2	3:D:743:ASP:OD2	2.47	0.48
2:C:193:LEU:HD21	2:C:307:LEU:HD21	1.96	0.48
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.96	0.48
3:D:433:GLY:HA3	3:D:447:VAL:O	2.13	0.48
1:B:57:TYR:CD2	1:B:161:ARG:HG3	2.49	0.48
1:B:100:LEU:HD23	1:B:141:GLU:HB3	1.95	0.48
2:C:1008:ARG:HH21	2:C:1020:PRO:HB3	1.78	0.48
3:D:417:PRO:HG3	3:D:431:VAL:HA	1.96	0.48
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.14	0.48
3:D:832:ARG:O	3:D:834:THR:N	2.47	0.48
3:D:704:ARG:HG2	3:D:736:PHE:O	2.14	0.47
3:D:1349:VAL:HG22	3:D:1368:ILE:HG22	1.96	0.47
2:C:45:GLN:O	2:C:48:PHE:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:607:LEU:HD23	3:D:614:PHE:CE1	2.48	0.47
3:D:1258:ARG:HG3	3:D:1258:ARG:HH11	1.78	0.47
3:D:1481:VAL:HG13	4:E:18:ARG:HA	1.96	0.47
4:E:51:LEU:HD23	4:E:51:LEU:H	1.78	0.47
2:C:19:THR:HG21	2:C:124:ASP:O	2.14	0.47
3:D:47:GLU:HG2	3:D:52:PRO:HA	1.95	0.47
3:D:543:LEU:HG	3:D:600:LEU:HD12	1.96	0.47
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.15	0.47
3:D:1309:ALA:HB1	3:D:1326:THR:HG23	1.96	0.47
2:C:162:ILE:HB	2:C:172:ILE:HB	1.96	0.47
2:C:1055:LEU:HD11	2:C:1066:ALA:HB2	1.97	0.47
3:D:1128:VAL:HG12	3:D:1129:THR:H	1.79	0.47
2:C:577:PRO:HB2	2:C:580:MET:HB3	1.97	0.47
3:D:190:GLU:HG2	3:D:196:VAL:HG22	1.96	0.47
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.29	0.47
2:C:274:ARG:NH1	2:C:284:ARG:HH22	2.10	0.47
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.49	0.47
2:C:971:LYS:HA	2:C:988:VAL:HA	1.95	0.47
3:D:100:ALA:HB2	3:D:513:ILE:HG13	1.95	0.47
3:D:1008:PHE:CZ	3:D:1032:PRO:HA	2.49	0.47
3:D:1165:TYR:HB3	3:D:1207:TYR:CE1	2.42	0.47
3:D:1261:GLU:OE2	3:D:1269:LYS:HG3	2.14	0.47
1:A:54:THR:HG21	1:A:158:ILE:HD12	1.97	0.47
3:D:212:ARG:HB3	3:D:388:HIS:CD2	2.49	0.47
3:D:474:GLU:O	3:D:478:LEU:HB2	2.14	0.47
3:D:565:ILE:O	3:D:569:ASN:HB2	2.14	0.47
3:D:890:VAL:O	3:D:926:LYS:NZ	2.48	0.47
3:D:1278:ASP:HA	3:D:1319:VAL:HG13	1.96	0.47
4:E:23:VAL:HG13	4:E:64:ALA:HB3	1.97	0.47
2:C:73:LEU:HB2	2:C:93:PRO:O	2.15	0.47
2:C:700:TYR:HB2	2:C:833:LEU:HB2	1.96	0.47
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.97	0.47
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.15	0.47
3:D:1315:ASP:OD2	3:D:1315:ASP:N	2.47	0.47
4:E:37:ASN:HB3	4:E:93:TYR:CZ	2.50	0.47
1:A:83:LYS:HD3	1:A:168:ASP:HB2	1.96	0.47
1:B:185:ARG:HH11	3:D:692:GLU:CD	2.18	0.47
3:D:46:ASP:OD2	3:D:48:ARG:HB3	2.15	0.47
3:D:853:VAL:HG11	3:D:860:LEU:HG	1.97	0.47
4:E:22:VAL:CG1	4:E:68:LEU:HD21	2.45	0.47
2:C:205:GLU:H	2:C:205:GLU:HG3	1.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:409:ARG:HA	2:C:454:SER:HA	1.95	0.46
3:D:82:LYS:C	3:D:84:ILE:H	2.18	0.46
3:D:185:VAL:CG2	3:D:203:ALA:HB2	2.46	0.46
3:D:565:ILE:HD12	3:D:565:ILE:N	2.30	0.46
3:D:989:TYR:O	3:D:993:LEU:HG	2.15	0.46
3:D:1106:VAL:HG11	3:D:1474:ALA:HB2	1.96	0.46
3:D:1282:ARG:HB2	3:D:1293:PHE:O	2.15	0.46
1:B:23:PHE:CD2	1:B:211:LEU:HD22	2.50	0.46
1:B:185:ARG:HD3	3:D:692:GLU:OE2	2.13	0.46
3:D:28:LYS:C	3:D:548:ILE:HG21	2.35	0.46
3:D:808:THR:H	3:D:809:PRO:CD	2.17	0.46
2:C:1051:GLU:OE1	3:D:752:SER:HB3	2.15	0.46
3:D:1272:ALA:O	3:D:1325:LEU:HD23	2.15	0.46
2:C:475:VAL:O	2:C:477:GLY:N	2.48	0.46
2:C:744:ARG:HH11	2:C:747:ALA:HB2	1.79	0.46
2:C:1073:GLY:HA3	3:D:659:LYS:HG2	1.97	0.46
3:D:560:GLN:HG3	3:D:561:GLY:H	1.79	0.46
3:D:1112:CYS:HB2	3:D:1195:GLN:HG2	1.98	0.46
1:B:11:PHE:CE1	1:B:23:PHE:HB3	2.51	0.46
2:C:1051:GLU:OE2	3:D:751:LEU:HB2	2.15	0.46
3:D:355:VAL:HG11	3:D:385:VAL:HG11	1.98	0.46
2:C:255:ALA:HB1	2:C:298:PHE:HE1	1.80	0.46
2:C:260:LEU:HG	2:C:291:ALA:HB3	1.98	0.46
1:B:42:ARG:HH22	2:C:939:ARG:NH2	2.14	0.46
2:C:838:LYS:HE3	3:D:741:ASP:O	2.15	0.46
2:C:949:LYS:HD3	3:D:796:ARG:NH1	2.31	0.46
3:D:65:ARG:HD2	3:D:65:ARG:HA	1.65	0.46
3:D:539:ASP:HB3	3:D:600:LEU:HB3	1.97	0.46
3:D:602:SER:O	3:D:606:ILE:HG12	2.15	0.46
3:D:978:TYR:HB2	3:D:983:LEU:HD11	1.97	0.46
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.16	0.46
3:D:1422:MET:HB2	3:D:1426:LYS:HD3	1.97	0.46
1:A:89:PHE:HE1	1:A:97:VAL:HB	1.79	0.46
2:C:676:ILE:HG23	2:C:988:VAL:HG13	1.97	0.46
2:C:726:ILE:HD12	2:C:734:LEU:HD11	1.97	0.46
2:C:892:LEU:HD23	2:C:918:LEU:HD22	1.98	0.46
3:D:179:VAL:HG11	3:D:203:ALA:HB3	1.96	0.46
3:D:214:GLU:HB3	3:D:340:THR:OG1	2.15	0.46
3:D:1018:ASN:HD21	3:D:1020:LEU:HB3	1.81	0.46
3:D:1119:SER:HB2	3:D:1185:GLU:HB3	1.97	0.46
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:288:ARG:HD3	2:C:288:ARG:H	1.81	0.46
2:C:715:THR:OG1	2:C:718:GLY:O	2.34	0.46
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.98	0.46
3:D:57:GLU:HG2	3:D:58:CYS:N	2.30	0.46
3:D:352:ASN:ND2	3:D:371:ILE:HG12	2.30	0.46
3:D:1197:ARG:HB3	3:D:1396:GLU:CD	2.37	0.46
2:C:15:LEU:O	2:C:586:ARG:NH2	2.49	0.45
2:C:260:LEU:O	2:C:262:ALA:N	2.45	0.45
2:C:358:ARG:HD3	2:C:372:LEU:HA	1.98	0.45
2:C:957:LYS:HD3	2:C:961:GLU:HB3	1.98	0.45
3:D:81:THR:HG22	3:D:82:LYS:H	1.81	0.45
1:B:186:LEU:O	1:B:188:GLN:NE2	2.50	0.45
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.97	0.45
3:D:63:TYR:HB3	3:D:68:PHE:CE1	2.51	0.45
3:D:613:ARG:NH1	3:D:616:GLN:HG2	2.30	0.45
3:D:709:HIS:ND1	3:D:1231:GLU:HG3	2.32	0.45
3:D:739:ASP:OD2	3:D:741:ASP:OD2	2.33	0.45
3:D:1388:ARG:HD2	3:D:1388:ARG:N	2.31	0.45
3:D:1435:LEU:HB2	3:D:1464:GLU:HG3	1.98	0.45
1:A:49:PRO:HA	1:A:148:VAL:HG22	1.99	0.45
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.98	0.45
2:C:274:ARG:HG2	2:C:285:LEU:HB3	1.98	0.45
3:D:86:ARG:O	3:D:522:PRO:HD2	2.16	0.45
3:D:416:ALA:HB3	3:D:419:ASP:OD1	2.17	0.45
3:D:792:ILE:HD13	3:D:941:PHE:HD2	1.82	0.45
3:D:1136:LYS:HB3	3:D:1139:ASP:OD2	2.16	0.45
3:D:1310:ARG:NH1	3:D:1327:ARG:NH1	2.65	0.45
3:D:1371:VAL:O	3:D:1375:MET:HG3	2.16	0.45
4:E:45:ARG:HH21	4:E:63:TRP:HH2	1.63	0.45
2:C:431:HIS:N	2:C:434:HIS:HD2	2.15	0.45
3:D:554:LEU:HD13	3:D:570:GLU:HB3	1.99	0.45
3:D:800:LYS:HG2	3:D:804:LEU:HD22	1.98	0.45
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.97	0.45
2:C:196:LEU:HA	2:C:199:VAL:HG23	1.97	0.45
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.99	0.45
2:C:1109:VAL:HG22	3:D:2:LYS:HB2	1.99	0.45
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.52	0.45
3:D:583:ASP:OD2	3:D:604:THR:HG21	2.17	0.45
2:C:642:ARG:NE	2:C:657:ASP:OD2	2.50	0.45
3:D:41:ARG:HE	3:D:41:ARG:HB3	1.59	0.45
3:D:496:LEU:HD21	3:D:1388:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.99	0.45
3:D:939:PHE:O	3:D:943:THR:HG23	2.17	0.45
7:T:2:DG:H2"	7:T:3:DG:C8	2.52	0.45
2:C:98:LEU:HD12	2:C:99:GLN:N	2.32	0.45
2:C:512:ARG:HD3	2:C:512:ARG:HA	1.77	0.45
2:C:842:ARG:HH11	2:C:842:ARG:HB3	1.81	0.45
3:D:527:MET:SD	3:D:537:THR:HB	2.57	0.45
3:D:978:TYR:HB2	3:D:988:ARG:HD3	1.99	0.45
3:D:1044:LEU:HD23	3:D:1044:LEU:H	1.82	0.45
3:D:1294:VAL:HG12	3:D:1295:GLU:N	2.31	0.45
4:E:22:VAL:HG11	4:E:68:LEU:HD21	1.97	0.45
2:C:281:LEU:HD13	2:C:281:LEU:H	1.82	0.45
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.99	0.45
3:D:39:PRO:HD3	3:D:53:ILE:HG21	1.99	0.45
3:D:53:ILE:HA	3:D:86:ARG:HH11	1.82	0.45
2:C:69:LEU:O	2:C:97:ARG:HB2	2.17	0.45
2:C:572:ILE:HG13	2:C:573:ARG:H	1.82	0.45
3:D:660:LYS:O	3:D:664:LYS:HG3	2.16	0.45
3:D:1283:ILE:HG13	3:D:1292:VAL:HG22	1.98	0.45
1:A:169:ALA:HB1	1:A:171:PHE:CE2	2.52	0.45
2:C:393:GLN:HG2	6:R:25:G:O2'	2.16	0.45
2:C:77:PRO:HD2	2:C:91:GLN:O	2.16	0.44
2:C:284:ARG:CG	2:C:301:GLU:HG2	2.47	0.44
2:C:1031:ARG:HB3	7:T:16:DC:OP1	2.17	0.44
2:C:225:SER:O	2:C:229:MET:HB2	2.16	0.44
2:C:431:HIS:CG	2:C:432:ARG:N	2.85	0.44
3:D:168:THR:HA	3:D:394:LEU:HB3	1.99	0.44
2:C:722:ILE:HA	2:C:758:ARG:HB3	1.99	0.44
2:C:974:LEU:HD12	2:C:974:LEU:HA	1.84	0.44
3:D:1149:LEU:HD21	3:D:1166:LEU:HD11	1.99	0.44
3:D:1294:VAL:O	3:D:1295:GLU:HB2	2.17	0.44
1:A:70:GLY:HA2	1:A:133:GLU:HB3	1.99	0.44
2:C:144:PRO:O	2:C:276:LYS:NZ	2.34	0.44
3:D:829:VAL:O	3:D:831:GLY:N	2.47	0.44
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.99	0.44
3:D:1394:VAL:HG21	3:D:1432:LYS:NZ	2.32	0.44
3:D:1435:LEU:HD23	3:D:1464:GLU:O	2.16	0.44
2:C:387:SER:OG	2:C:388:ARG:NH2	2.50	0.44
2:C:743:VAL:HG11	2:C:755:LEU:HD12	2.00	0.44
3:D:616:GLN:HG3	3:D:621:LYS:HZ3	1.83	0.44
1:A:133:GLU:OE2	2:C:605:LYS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:THR:HG22	1:B:202:ASP:H	1.83	0.44
2:C:397:GLU:HG2	2:C:403:SER:OG	2.18	0.44
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.99	0.44
2:C:675:ALA:HB2	2:C:867:VAL:HG21	1.99	0.44
2:C:724:ARG:HB2	2:C:741:GLY:H	1.83	0.44
3:D:11:ALA:HA	3:D:1451:ALA:O	2.17	0.44
3:D:205:TYR:CD1	3:D:390:PRO:HG3	2.53	0.44
3:D:808:THR:N	3:D:809:PRO:HD2	2.18	0.44
1:B:208:LEU:HD13	1:B:208:LEU:HA	1.86	0.44
2:C:274:ARG:HH22	2:C:284:ARG:NH2	2.16	0.44
2:C:295:ASP:C	2:C:297:GLU:H	2.20	0.44
2:C:468:ARG:NE	2:C:485:TYR:O	2.51	0.44
2:C:1017:THR:OG1	2:C:1019:GLN:HG2	2.17	0.44
4:E:47:LYS:HB3	4:E:55:PHE:HE2	1.83	0.44
2:C:141:HIS:CE1	2:C:334:ARG:HG3	2.52	0.44
3:D:353:VAL:HG22	3:D:368:VAL:HG22	1.99	0.44
3:D:825:ALA:HA	3:D:826:PRO:HD2	1.88	0.44
3:D:961:LYS:O	3:D:965:GLU:HB2	2.18	0.44
3:D:1127:GLU:HB3	3:D:1133:ARG:CZ	2.48	0.44
2:C:108:ILE:HG13	2:C:366:SER:HB2	2.00	0.43
2:C:468:ARG:HD3	2:C:485:TYR:HB3	1.99	0.43
3:D:553:ARG:NH2	3:D:570:GLU:OE2	2.51	0.43
3:D:1314:LYS:HZ1	3:D:1316:GLY:HA3	1.83	0.43
3:D:1466:VAL:HG22	3:D:1472:ILE:HG22	2.00	0.43
2:C:64:LEU:HD13	2:C:359:MET:SD	2.58	0.43
2:C:727:PRO:HG2	2:C:759:THR:HG21	1.99	0.43
3:D:796:ARG:HB2	3:D:828:LYS:HG2	2.00	0.43
3:D:1301:LYS:HD2	3:D:1303:TYR:CE1	2.54	0.43
1:A:122:ILE:HG22	1:A:124:ASN:H	1.84	0.43
2:C:100:LEU:HB3	2:C:368:THR:OG1	2.19	0.43
2:C:250:ARG:O	2:C:254:VAL:HG23	2.18	0.43
2:C:842:ARG:HH11	2:C:842:ARG:CB	2.31	0.43
2:C:1023:GLY:HA2	2:C:1026:GLN:O	2.19	0.43
3:D:708:LEU:HD21	3:D:1091:SER:HB2	1.99	0.43
3:D:1280:VAL:HG23	3:D:1282:ARG:HG3	2.00	0.43
3:D:1314:LYS:HZ2	3:D:1316:GLY:HA3	1.81	0.43
2:C:2:GLU:HG3	2:C:899:GLN:HB3	1.99	0.43
2:C:13:ILE:HA	2:C:14:PRO:HD3	1.90	0.43
2:C:658:GLY:N	2:C:661:SER:HG	2.14	0.43
3:D:58:CYS:HA	3:D:78:VAL:HG11	2.01	0.43
3:D:414:ARG:HG3	3:D:433:GLY:N	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:26:U:H2'	6:R:27:G:H8	1.84	0.43
1:B:186:LEU:O	1:B:188:GLN:N	2.52	0.43
2:C:54:ILE:CG2	2:C:66:LEU:HD23	2.49	0.43
2:C:146:VAL:HA	2:C:161:SER:O	2.18	0.43
2:C:1019:GLN:HA	2:C:1020:PRO:HD3	1.76	0.43
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.52	0.43
2:C:1076:VAL:HB	3:D:752:SER:HA	2.00	0.43
3:D:465:LEU:HD22	3:D:509:PRO:HB2	1.99	0.43
3:D:966:GLU:HA	3:D:969:ARG:HG2	2.00	0.43
3:D:1295:GLU:HB3	3:D:1296:SER:H	1.49	0.43
4:E:38:THR:HG23	4:E:41:GLU:HG2	2.01	0.43
1:A:32:PHE:CE2	1:B:43:ILE:HG12	2.54	0.43
2:C:56:GLU:HB2	2:C:64:LEU:HB3	2.00	0.43
2:C:358:ARG:HD3	2:C:371:LYS:O	2.19	0.43
2:C:700:TYR:HB3	2:C:996:LYS:HE3	2.00	0.43
3:D:178:LEU:HD13	3:D:178:LEU:HA	1.83	0.43
3:D:458:ALA:HB2	3:D:575:GLN:NE2	2.33	0.43
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.99	0.43
3:D:1312:LEU:HD11	3:D:1327:ARG:HE	1.82	0.43
3:D:1381:VAL:HG23	3:D:1391:GLU:O	2.19	0.43
6:R:22:U:H2'	6:R:23:G:H8	1.82	0.43
3:D:1412:LYS:C	3:D:1414:PRO:HD3	2.39	0.43
1:B:59:GLU:HB3	1:B:137:ARG:NH1	2.31	0.43
2:C:434:HIS:ND1	2:C:438:ILE:HD12	2.34	0.43
2:C:540:PHE:CE2	2:C:906:PHE:HE2	2.37	0.43
3:D:32:ILE:HG21	3:D:37:LEU:HD13	2.01	0.43
3:D:1277:ILE:HG13	3:D:1301:LYS:HZ3	1.82	0.43
1:B:153:ALA:HB2	1:B:168:ASP:N	2.34	0.43
3:D:15:PRO:HB3	3:D:19:ARG:HH22	1.83	0.43
3:D:24:GLY:HA3	3:D:49:ILE:HG12	1.99	0.43
3:D:760:ARG:NH2	4:E:3:GLU:OE1	2.46	0.43
2:C:136:ILE:HD11	2:C:386:PHE:CE1	2.54	0.42
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.52	0.42
3:D:123:LEU:HG	3:D:152:LEU:HD21	2.00	0.42
3:D:148:GLU:OE2	3:D:153:LEU:HD22	2.18	0.42
3:D:462:GLN:O	3:D:466:LYS:HG3	2.19	0.42
1:A:32:PHE:CZ	1:B:43:ILE:HG12	2.54	0.42
1:A:89:PHE:HB3	1:A:94:LEU:HD12	2.01	0.42
2:C:56:GLU:HA	2:C:356:ARG:HH12	1.84	0.42
2:C:355:VAL:HG23	2:C:372:LEU:HB3	2.01	0.42
2:C:542:VAL:HA	2:C:545:ASN:HB2	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:565:GLN:H	2:C:565:GLN:HG2	1.64	0.42
2:C:1008:ARG:HD3	2:C:1028:GLY:N	2.35	0.42
3:D:729:HIS:HE2	3:D:935:LYS:HD2	1.84	0.42
3:D:908:LYS:HB2	3:D:1027:GLY:HA3	2.01	0.42
1:B:20:TYR:HA	1:B:199:ILE:O	2.19	0.42
2:C:603:VAL:HB	2:C:647:GLN:H	1.84	0.42
2:C:1016:ILE:HG13	2:C:1017:THR:HG22	2.00	0.42
3:D:176:ASP:HB3	3:D:177:ALA:H	1.55	0.42
3:D:908:LYS:HB2	3:D:1027:GLY:CA	2.48	0.42
3:D:968:ASP:HA	3:D:971:LEU:HD23	2.01	0.42
3:D:1325:LEU:HD22	3:D:1325:LEU:H	1.84	0.42
4:E:3:GLU:HB2	4:E:6:ILE:CG2	2.50	0.42
1:B:11:PHE:HE1	1:B:23:PHE:HB3	1.84	0.42
2:C:274:ARG:HB2	2:C:285:LEU:HD22	2.01	0.42
2:C:891:GLY:O	2:C:991:GLN:HG2	2.20	0.42
3:D:952:ASP:HA	3:D:1062:ARG:HH11	1.84	0.42
4:E:57:ASP:N	4:E:58:PRO:HD3	2.35	0.42
1:A:24:VAL:HG22	1:A:196:THR:HG22	2.01	0.42
1:A:57:TYR:CD2	1:A:161:ARG:HG3	2.54	0.42
1:A:143:ARG:NH1	1:A:158:ILE:HG21	2.35	0.42
2:C:442:GLU:OE2	2:C:543:ASN:ND2	2.43	0.42
2:C:1103:ASP:HB3	2:C:1105:LYS:HZ2	1.79	0.42
2:C:1105:LYS:H	2:C:1105:LYS:HD3	1.84	0.42
3:D:57:GLU:HG3	3:D:64:LYS:HD2	2.02	0.42
3:D:131:LYS:HB2	3:D:568:ARG:HG2	2.01	0.42
3:D:157:GLU:HA	3:D:160:GLU:HG2	2.01	0.42
3:D:983:LEU:H	3:D:983:LEU:HG	1.60	0.42
2:C:238:LEU:HD21	2:C:242:LEU:HD13	2.02	0.42
2:C:425:PHE:H	2:C:428:ARG:HD2	1.84	0.42
2:C:1046:ALA:HB2	3:D:1472:ILE:HG13	2.02	0.42
2:C:1073:GLY:CA	3:D:659:LYS:HG2	2.50	0.42
3:D:206:ARG:HG2	3:D:392:SER:HB2	2.01	0.42
3:D:462:GLN:HG2	3:D:466:LYS:HE3	2.02	0.42
4:E:9:LEU:HD23	4:E:19:LEU:HD11	2.00	0.42
7:T:13:DC:H2"	7:T:14:DA:OP2	2.18	0.42
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.91	0.42
1:A:84:GLU:O	1:A:124:ASN:ND2	2.52	0.42
2:C:846:LYS:NZ	6:R:29:U:P	2.90	0.42
2:C:1094:ALA:HB2	3:D:520:LEU:HD12	2.02	0.42
3:D:807:ALA:HA	3:D:833:GLU:CD	2.40	0.42
3:D:904:VAL:HB	3:D:905:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1301:LYS:HD3	3:D:1301:LYS:HA	1.94	0.42
2:C:344:PHE:CE1	2:C:378:LEU:HD11	2.55	0.42
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.54	0.42
3:D:466:LYS:HG2	3:D:510:GLU:HB3	2.02	0.42
3:D:1462:LEU:O	3:D:1465:ASN:N	2.53	0.42
5:N:7:DG:H2"	5:N:8:DA:C8	2.54	0.42
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.40	0.42
2:C:148:PHE:CE2	2:C:309:TYR:HD2	2.38	0.42
2:C:267:TYR:CB	2:C:272:ALA:HB3	2.50	0.42
3:D:841:TYR:HB3	3:D:843:PHE:CZ	2.55	0.42
3:D:1398:TRP:CE3	3:D:1398:TRP:HA	2.55	0.42
1:A:128:HIS:NE2	1:A:131:THR:HG23	2.35	0.42
1:B:18:ARG:NH2	1:B:203:GLY:O	2.49	0.42
2:C:216:GLU:C	2:C:218:VAL:H	2.22	0.42
2:C:810:ASP:HB2	2:C:813:VAL:HG13	2.02	0.42
2:C:889:HIS:O	2:C:918:LEU:HD21	2.20	0.42
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.94	0.42
3:D:568:ARG:HA	3:D:571:LYS:HG3	2.01	0.42
4:E:47:LYS:HA	4:E:54:LEU:HB3	2.01	0.42
7:T:3:DG:H2"	7:T:4:DA:C8	2.55	0.42
1:A:178:ALA:HB2	2:C:864:GLY:CA	2.50	0.41
2:C:272:ALA:HB1	2:C:276:LYS:HZ1	1.85	0.41
2:C:910:LYS:O	2:C:914:ILE:HG12	2.20	0.41
3:D:131:LYS:HG3	3:D:568:ARG:HG2	2.02	0.41
3:D:832:ARG:HA	3:D:832:ARG:HD2	1.74	0.41
3:D:1042:ARG:NH1	3:D:1073:SER:HB3	2.35	0.41
2:C:9:ILE:HG12	2:C:907:ASP:OD2	2.19	0.41
2:C:301:GLU:O	2:C:305:PRO:HD2	2.21	0.41
2:C:759:THR:HB	2:C:785:VAL:HG22	2.02	0.41
2:C:1008:ARG:NH1	2:C:1011:GLY:N	2.59	0.41
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.01	0.41
2:C:1038:TRP:HH2	3:D:1096:ARG:HA	1.85	0.41
3:D:881:LEU:O	3:D:885:ILE:HG13	2.20	0.41
3:D:1280:VAL:O	3:D:1294:VAL:HG13	2.20	0.41
2:C:118:ILE:HA	2:C:119:PRO:HD3	1.80	0.41
2:C:181:VAL:HA	2:C:220:GLY:O	2.20	0.41
2:C:352:ALA:O	2:C:355:VAL:HG12	2.20	0.41
2:C:473:ARG:HB2	2:C:473:ARG:NH1	2.35	0.41
3:D:29:PRO:HB3	3:D:548:ILE:HB	2.01	0.41
3:D:1401:GLU:CD	3:D:1415:VAL:HG22	2.40	0.41
4:E:80:VAL:HG11	4:E:85:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HB3	1:A:119:ASP:HB3	2.03	0.41
1:A:183:ASP:OD1	1:A:183:ASP:N	2.53	0.41
2:C:334:ARG:HH11	2:C:418:LEU:CD1	2.34	0.41
2:C:560:MET:HE3	2:C:846:LYS:HD3	2.02	0.41
2:C:1056:LYS:HB3	3:D:624:ASP:HB2	2.03	0.41
2:C:1103:ASP:N	2:C:1107:ASN:O	2.53	0.41
3:D:357:GLU:OE2	3:D:386:HIS:ND1	2.37	0.41
3:D:877:PRO:HA	3:D:880:ILE:HG22	2.02	0.41
2:C:36:PRO:HB2	2:C:70:GLU:CD	2.41	0.41
2:C:327:HIS:CE1	2:C:489:THR:HA	2.56	0.41
2:C:724:ARG:HB2	2:C:741:GLY:N	2.36	0.41
2:C:1101:THR:HG21	2:C:1111:ILE:HD11	2.02	0.41
3:D:32:ILE:HG22	3:D:33:ASN:O	2.20	0.41
3:D:1289:LYS:NZ	3:D:1304:LYS:HB2	2.36	0.41
1:A:67:THR:HB	2:C:627:ARG:HD3	2.02	0.41
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.56	0.41
2:C:969:GLN:HG2	3:D:952:ASP:OD2	2.21	0.41
3:D:161:LEU:HD23	3:D:162:ARG:HG2	2.02	0.41
3:D:426:LYS:HE2	3:D:426:LYS:HB3	1.90	0.41
3:D:1291:SER:HA	3:D:1302:GLU:OE2	2.20	0.41
3:D:1412:LYS:HD3	3:D:1412:LYS:HA	1.47	0.41
1:B:11:PHE:HB2	1:B:25:LEU:HD12	2.02	0.41
2:C:246:ASP:HA	2:C:247:PRO:HD3	1.70	0.41
2:C:749:VAL:HA	2:C:753:ASP:OD2	2.19	0.41
2:C:1105:LYS:HZ3	2:C:1107:ASN:HB2	1.84	0.41
3:D:568:ARG:HA	3:D:568:ARG:HD2	1.97	0.41
3:D:764:LEU:O	3:D:768:ASN:ND2	2.45	0.41
3:D:1004:THR:HG23	3:D:1036:ARG:HB2	2.03	0.41
4:E:41:GLU:H	4:E:41:GLU:HG3	1.56	0.41
7:T:11:DT:H2"	7:T:12:DC:O5'	2.21	0.41
2:C:572:ILE:HG13	2:C:573:ARG:N	2.35	0.41
3:D:31:THR:HG1	3:D:32:ILE:H	1.68	0.41
3:D:1142:ALA:HB1	3:D:1364:HIS:HA	2.03	0.41
3:D:1290:LEU:HD21	3:D:1305:LEU:HD13	2.02	0.41
7:T:4:DA:H2"	7:T:5:DA:C8	2.56	0.41
1:A:46:SER:OG	1:A:47:SER:N	2.52	0.41
1:A:141:GLU:OE1	1:A:141:GLU:N	2.53	0.41
1:A:151:VAL:HA	1:A:152:PRO:HD2	1.93	0.41
1:B:77:GLU:OE2	3:D:867:ARG:NH1	2.54	0.41
2:C:78:PHE:HA	2:C:79:PRO:HD3	1.88	0.41
2:C:137:VAL:HG23	2:C:391:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:GLU:HG2	2:C:178:PRO:HD2	2.03	0.41
2:C:214:TYR:HD1	2:C:215:GLY:H	1.69	0.41
3:D:704:ARG:HG3	3:D:705:ALA:N	2.36	0.41
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.03	0.41
3:D:1407:LEU:HD23	3:D:1407:LEU:HA	1.91	0.41
3:D:1458:GLU:O	3:D:1460:ILE:HG22	2.20	0.41
3:D:1492:LEU:O	3:D:1496:GLU:HB2	2.21	0.41
4:E:26:ARG:NH1	4:E:73:LEU:HD21	2.35	0.41
5:N:3:DA:H2"	5:N:4:DA:C8	2.56	0.41
6:R:26:U:H2'	6:R:27:G:C8	2.56	0.41
1:B:56:VAL:HG23	1:B:167:VAL:HG21	2.02	0.41
2:C:73:LEU:HD22	2:C:94:LEU:HA	2.03	0.41
2:C:1071:ILE:HD13	2:C:1071:ILE:HA	1.90	0.41
3:D:1197:ARG:HH21	3:D:1198:TYR:HE2	1.69	0.41
2:C:378:LEU:O	2:C:382:ILE:HG12	2.21	0.40
2:C:682:TYR:HA	3:D:633:VAL:HG11	2.02	0.40
3:D:108:VAL:HB	3:D:109:PRO:HD3	2.02	0.40
3:D:470:LEU:H	3:D:470:LEU:HG	1.69	0.40
1:A:26:GLU:OE2	1:A:185:ARG:HB2	2.21	0.40
2:C:219:GLN:O	2:C:223:ASP:OD2	2.38	0.40
2:C:257:VAL:O	2:C:264:PRO:HD3	2.21	0.40
3:D:465:LEU:HD13	3:D:509:PRO:O	2.22	0.40
3:D:629:SER:OG	3:D:630:VAL:N	2.55	0.40
3:D:983:LEU:CD1	3:D:988:ARG:HB2	2.44	0.40
1:A:42:ARG:HE	2:C:856:GLU:HB2	1.84	0.40
1:A:86:VAL:HG21	1:A:202:ASP:HB2	2.04	0.40
1:A:100:LEU:HD22	1:A:141:GLU:HG3	2.02	0.40
1:A:214:ALA:HA	1:A:217:ILE:HD12	2.03	0.40
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.56	0.40
3:D:834:THR:HB	3:D:838:ARG:HD2	2.04	0.40
3:D:1310:ARG:HH11	3:D:1327:ARG:NH1	2.20	0.40
3:D:1311:LEU:HA	3:D:1325:LEU:O	2.20	0.40
5:N:6:DA:H2"	5:N:7:DG:C8	2.56	0.40
2:C:184:MET:O	2:C:190:LYS:HA	2.21	0.40
2:C:442:GLU:HG2	2:C:454:SER:CB	2.51	0.40
3:D:801:GLY:HA3	3:D:826:PRO:HD2	2.04	0.40
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:NH1	3:D:1297:GLU:OE2[3_455]	2.18	0.02

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	221/315 (70%)	186 (84%)	29 (13%)	6 (3%)	5 34
1	B	221/315 (70%)	193 (87%)	25 (11%)	3 (1%)	11 47
2	C	1077/1119 (96%)	897 (83%)	144 (13%)	36 (3%)	4 30
3	D	1352/1534 (88%)	1097 (81%)	198 (15%)	57 (4%)	3 25
4	E	91/99 (92%)	73 (80%)	13 (14%)	5 (6%)	2 21
All	All	2962/3382 (88%)	2446 (83%)	409 (14%)	107 (4%)	3 28

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	184	THR
2	C	2	GLU
2	C	111	ASP
2	C	164	PRO
2	C	213	ALA
2	C	217	LEU
2	C	262	ALA
3	D	117	ASP
3	D	165	LYS
3	D	176	ASP
3	D	363	ALA
3	D	705	ALA
3	D	808	THR
3	D	823	LEU
3	D	1067	VAL

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Mol	Chain	Res	Type
3	D	1273	VAL
3	D	1294	VAL
3	D	1295	GLU
3	D	1327	ARG
3	D	1433	SER
3	D	1454	GLY
3	D	1459	LEU
1	A	29	GLU
2	C	96	ALA
2	C	114	PHE
2	C	248	PRO
2	C	320	HIS
2	C	476	GLY
2	C	517	ARG
2	C	984	GLU
3	D	55	ASP
3	D	82	LYS
3	D	137	PRO
3	D	594	PRO
3	D	824	ASN
3	D	1205	TYR
1	A	48	ILE
1	B	125	PRO
2	C	231	PRO
2	C	244	PRO
2	C	274	ARG
2	C	367	LEU
2	C	542	VAL
2	C	815	LEU
3	D	164	GLY
3	D	200	ASP
3	D	345	TYR
3	D	374	GLU
3	D	417	PRO
3	D	560	GLN
3	D	616	GLN
3	D	806	PHE
3	D	830	ALA
3	D	844	ALA
3	D	1128	VAL
3	D	1284	GLU
3	D	1287	GLU

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Mol	Chain	Res	Type
3	D	1302	GLU
4	E	4	PRO
4	E	42	PRO
4	E	50	THR
1	A	186	LEU
2	C	33	ASP
2	C	187	ASN
2	C	188	LYS
2	C	315	ALA
2	C	864	GLY
3	D	406	ASP
3	D	425	GLY
3	D	832	ARG
3	D	1129	THR
3	D	1269	LYS
3	D	1385	GLY
2	C	39	ARG
2	C	369	PRO
2	C	680	ASP
2	C	795	GLY
3	D	410	SER
3	D	522	PRO
3	D	722	GLU
3	D	1317	ASP
2	C	272	ALA
2	C	999	HIS
3	D	146	PRO
3	D	601	ARG
3	D	735	ALA
3	D	1197	ARG
4	E	58	PRO
1	B	187	GLY
2	C	905	ILE
3	D	182	GLY
3	D	1032	PRO
2	C	52	PHE
2	C	152	PRO
2	C	983	ILE
3	D	109	PRO
3	D	1155	VAL
3	D	1411	GLY
1	B	158	ILE

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Mol	Chain	Res	Type
3	D	208	PRO
3	D	1306	PRO
2	C	376	ARG
4	E	41	GLU
1	A	109	VAL
2	C	261	ILE
3	D	809	PRO

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	196/273 (72%)	188 (96%)	8 (4%)	30	56
1	B	196/273 (72%)	189 (96%)	7 (4%)	35	60
2	C	912/941 (97%)	837 (92%)	75 (8%)	11	37
3	D	1147/1289 (89%)	1044 (91%)	103 (9%)	9	33
4	E	82/88 (93%)	70 (85%)	12 (15%)	3	18
All	All	2533/2864 (88%)	2328 (92%)	205 (8%)	11	38

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	12	THR
1	A	15	THR
1	A	32	PHE
1	A	46	SER
1	A	126	ASP
1	A	165	ILE
1	A	182	GLU
1	B	26	GLU
1	B	63	HIS
1	B	112	ARG
1	B	201	THR

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Mol	Chain	Res	Type
1	B	205	VAL
1	B	206	THR
1	B	208	LEU
2	C	8	ARG
2	C	26	TYR
2	C	30	LEU
2	C	39	ARG
2	C	49	ARG
2	C	52	PHE
2	C	81	ASP
2	C	98	LEU
2	C	104	ASP
2	C	118	ILE
2	C	127	PHE
2	C	135	VAL
2	C	154	ARG
2	C	157	ARG
2	C	189	ARG
2	C	193	LEU
2	C	205	GLU
2	C	214	TYR
2	C	223	ASP
2	C	232	GLU
2	C	267	TYR
2	C	268	ASP
2	C	274	ARG
2	C	281	LEU
2	C	284	ARG
2	C	288	ARG
2	C	289	THR
2	C	295	ASP
2	C	299	LYS
2	C	300	ASP
2	C	303	PHE
2	C	306	THR
2	C	307	LEU
2	C	321	GLU
2	C	350	ARG
2	C	367	LEU
2	C	375	SER
2	C	376	ARG
2	C	378	LEU

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Mol	Chain	Res	Type
2	C	388	ARG
2	C	391	LEU
2	C	393	GLN
2	C	394	PHE
2	C	402	SER
2	C	403	SER
2	C	405	ARG
2	C	420	ARG
2	C	473	ARG
2	C	481	ASP
2	C	506	ASN
2	C	567	GLN
2	C	610	ARG
2	C	620	LEU
2	C	626	ARG
2	C	627	ARG
2	C	699	PHE
2	C	703	ILE
2	C	728	HIS
2	C	810	ASP
2	C	835	VAL
2	C	842	ARG
2	C	865	THR
2	C	880	MET
2	C	899	GLN
2	C	907	ASP
2	C	953	VAL
2	C	966	LEU
2	C	978	ARG
2	C	995	MET
2	C	1000	MET
2	C	1001	VAL
2	C	1008	ARG
2	C	1021	LEU
2	C	1099	VAL
2	C	1105	LYS
3	D	5	VAL
3	D	41	ARG
3	D	58	CYS
3	D	60	CYS
3	D	64	LYS
3	D	68	PHE

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Mol	Chain	Res	Type
3	D	73	CYS
3	D	74	GLU
3	D	75	ARG
3	D	79	GLU
3	D	80	VAL
3	D	85	VAL
3	D	87	ARG
3	D	107	ASP
3	D	124	GLU
3	D	127	LEU
3	D	142	LEU
3	D	149	LYS
3	D	150	ARG
3	D	152	LEU
3	D	153	LEU
3	D	161	LEU
3	D	166	GLN
3	D	176	ASP
3	D	178	LEU
3	D	186	VAL
3	D	340	THR
3	D	347	VAL
3	D	372	ASP
3	D	382	GLU
3	D	400	VAL
3	D	435	VAL
3	D	449	SER
3	D	468	LEU
3	D	483	HIS
3	D	494	LYS
3	D	507	ASN
3	D	520	LEU
3	D	527	MET
3	D	550	ARG
3	D	642	CYS
3	D	686	GLU
3	D	724	GLN
3	D	734	GLU
3	D	754	PHE
3	D	783	ARG
3	D	800	LYS
3	D	804	LEU

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Mol	Chain	Res	Type
3	D	808	THR
3	D	813	LEU
3	D	817	GLU
3	D	823	LEU
3	D	828	LYS
3	D	833	GLU
3	D	892	ASP
3	D	902	LEU
3	D	932	ASP
3	D	935	LYS
3	D	971	LEU
3	D	983	LEU
3	D	991	GLN
3	D	1001	GLU
3	D	1012	GLU
3	D	1013	GLU
3	D	1029	ARG
3	D	1041	LEU
3	D	1044	LEU
3	D	1058	ARG
3	D	1070	TYR
3	D	1083	ASP
3	D	1094	LEU
3	D	1106	VAL
3	D	1109	GLU
3	D	1115	THR
3	D	1151	ARG
3	D	1162	GLU
3	D	1195	GLN
3	D	1197	ARG
3	D	1207	TYR
3	D	1209	LEU
3	D	1235	GLN
3	D	1262	LEU
3	D	1278	ASP
3	D	1296	SER
3	D	1299	PHE
3	D	1304	LYS
3	D	1305	LEU
3	D	1307	LYS
3	D	1314	LYS
3	D	1315	ASP

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Mol	Chain	Res	Type
3	D	1318	TYR
3	D	1325	LEU
3	D	1327	ARG
3	D	1342	GLU
3	D	1373	ARG
3	D	1389	LEU
3	D	1410	GLU
3	D	1412	LYS
3	D	1424	VAL
3	D	1433	SER
3	D	1441	GLN
3	D	1478	SER
3	D	1488	ASP
4	E	14	ASP
4	E	32	ARG
4	E	35	PHE
4	E	38	THR
4	E	39	VAL
4	E	41	GLU
4	E	47	LYS
4	E	49	GLN
4	E	51	LEU
4	E	56	ASP
4	E	57	ASP
4	E	74	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	B	156	HIS
2	C	141	HIS
2	C	406	HIS
2	C	431	HIS
2	C	434	HIS
2	C	609	ASN
2	C	884	GLN
3	D	388	HIS
3	D	462	GLN
3	D	1031	ASN
3	D	1033	GLN
3	D	1227	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	8/16 (50%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	22	U

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	223/315 (70%)	-0.18	2 (0%)	84	77	52, 116, 169, 205	0
1	B	223/315 (70%)	-0.20	1 (0%)	92	87	53, 107, 163, 198	0
2	C	1083/1119 (96%)	-0.20	5 (0%)	91	86	34, 108, 177, 264	0
3	D	1358/1534 (88%)	-0.12	25 (1%)	68	60	31, 110, 196, 250	0
4	E	93/99 (93%)	-0.05	1 (1%)	80	72	65, 121, 179, 228	0
5	N	11/13 (84%)	-0.21	0	100	100	340, 362, 386, 405	0
6	R	9/16 (56%)	-0.21	0	100	100	201, 206, 235, 243	0
7	T	22/22 (100%)	-0.46	0	100	100	219, 336, 388, 406	0
All	All	3022/3433 (88%)	-0.16	34 (1%)	80	72	31, 111, 192, 406	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	368	VAL	4.5
3	D	1299	PHE	4.0
2	C	372	LEU	3.5
3	D	1276	GLU	3.4
1	A	7	LYS	3.2
3	D	1290	LEU	3.2
3	D	1311	LEU	3.1
3	D	367	ILE	3.1
3	D	802	ALA	3.0
3	D	1303	TYR	2.9
2	C	373	VAL	2.8
3	D	355	VAL	2.8
3	D	1279	GLY	2.8
3	D	1321	ALA	2.7
3	D	1298	GLY	2.7
2	C	425	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	1278	ASP	2.5
3	D	1322	GLY	2.5
3	D	1269	LYS	2.5
3	D	44	LEU	2.5
3	D	393	ILE	2.5
2	C	1091	GLU	2.4
3	D	1410	GLU	2.4
1	B	64	GLU	2.4
3	D	1305	LEU	2.3
3	D	191	LEU	2.2
3	D	1297	GLU	2.2
4	E	57	ASP	2.2
3	D	949	ILE	2.2
2	C	833	LEU	2.2
3	D	1312	LEU	2.1
1	A	25	LEU	2.1
3	D	769	LEU	2.0
3	D	1263	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	ZN	D	1601	1/1	0.92	0.14	70,70,70,70	0
9	MG	D	1603	1/1	0.95	0.26	70,70,70,70	0
8	ZN	D	1602	1/1	0.99	0.28	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.