



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:52 PM GMT

PDB ID : 4Q5S
Title : Thermus thermophilus RNA polymerase initially transcribing complex containing 6-mer RNA
Authors : Murakami, K.S.
Deposited on : 2014-04-17
Resolution : 3.00 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

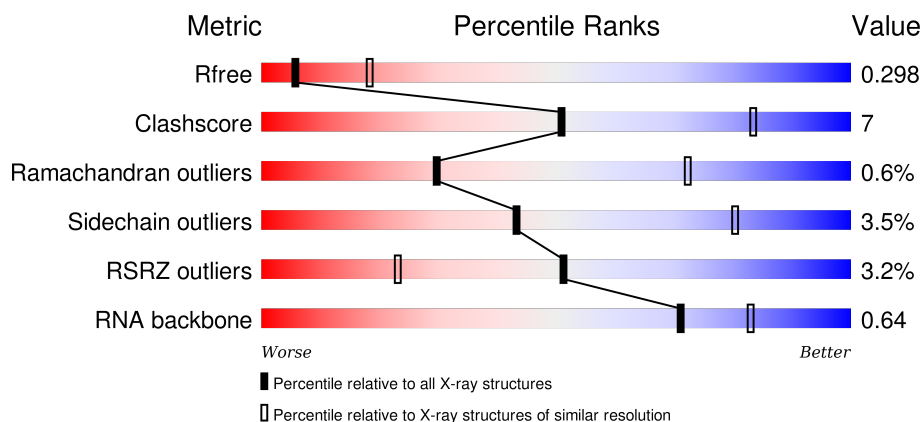
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	315	<div> <div>3%</div> <div>59%12%28%</div> </div>
1	B	315	<div> <div>60%9%30%</div> </div>
2	C	1119	<div> <div>3%</div> <div>79%20%..</div> </div>
3	D	1524	<div> <div>2%</div> <div>78%19%..</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>2%81%14%5%</div></div>
5	F	423	<div><div></div><div>8%62%16%20%</div></div>
6	G	22	<div><div></div><div>32%27%5%36%</div></div>
7	H	27	<div><div></div><div>37%22%41%</div></div>
8	I	5	<div><div></div><div>60%40%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28290 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1484	Total	C	N	O	S	0	0	0
			11722	7430	2064	2192	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	338	Total	C	N	O	S	0	0	0
			2747	1736	500	507	4			

- Molecule 6 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*AP*GP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	14	Total	C	N	O	P	0	0	0
			289	137	52	86	14			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	16	Total	C	N	O	P	0	0	0
			333	159	66	93	15			

- Molecule 8 is a RNA chain called RNA (5'-R(P*CP*UP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	5	Total	C	N	O	P	0	0	0
			102	46	16	35	5			

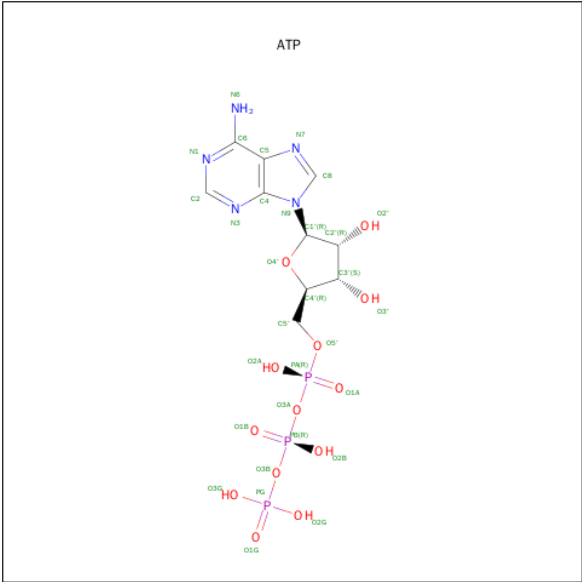
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

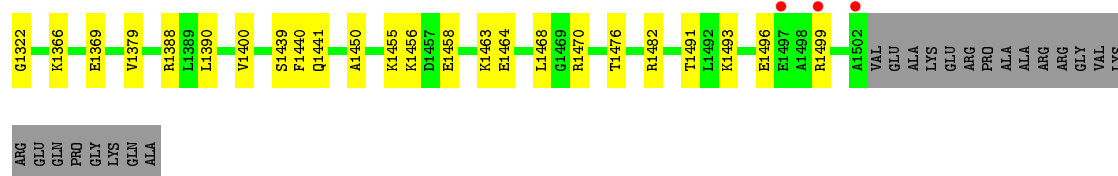
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

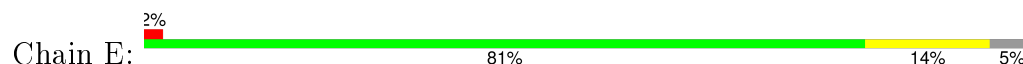
- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



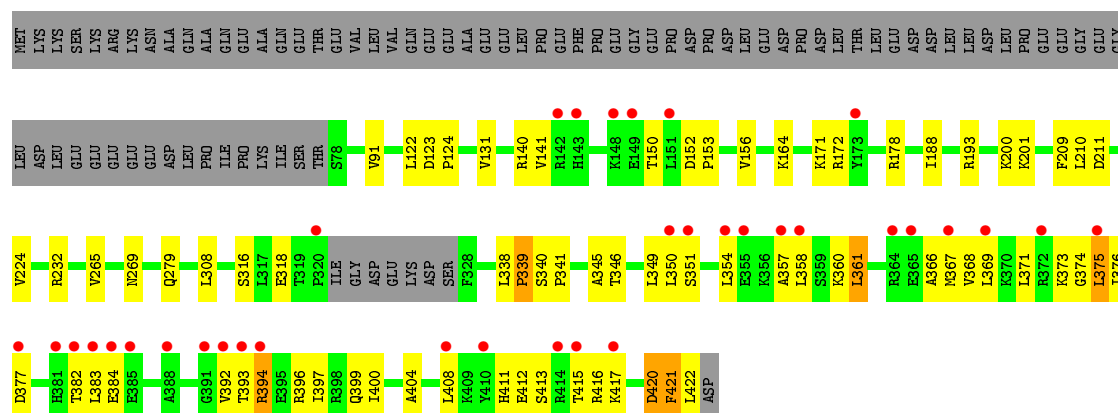
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		



- Molecule 4: DNA-directed RNA polymerase subunit omega



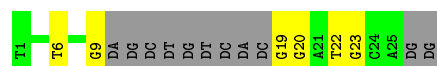
- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: DNA (5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*AP*GP*CP*CP*A)-3')



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3')



- Molecule 8: RNA (5'-R(P*CP*UP*CP*AP*C)-3')





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.09Å 102.08Å 297.26Å 90.00° 98.14° 90.00°	Depositor
Resolution (Å)	41.98 – 3.00 41.98 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.3 (41.98-3.00) 89.6 (41.98-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.269 , 0.294 0.280 , 0.298	Depositor DCC
R_{free} test set	1755 reflections (1.74%)	DCC
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 29.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 107824 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	28290	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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, ATP

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	0.21	0/1814	0.40	0/2466
1	B	0.21	0/1782	0.40	0/2424
2	C	0.21	0/8937	0.39	0/12087
3	D	0.21	0/11928	0.39	0/16127
4	E	0.21	0/775	0.38	0/1045
5	F	0.23	1/2791 (0.0%)	0.38	0/3754
6	G	0.55	0/323	1.02	1/497 (0.2%)
7	H	0.46	0/374	1.03	0/575
8	I	1.07	0/112	1.03	0/171
All	All	0.23	1/28836 (0.0%)	0.43	1/39146 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	339	PRO	C-N	-5.72	1.20	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	14	DG	O3'-P-O5'	-5.61	93.35	104.00

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	1782	0	1834	24	0
1	B	1750	0	1797	20	0
2	C	8770	0	8874	149	0
3	D	11722	0	11949	160	0
4	E	761	0	778	9	0
5	F	2747	0	2831	79	0
6	G	289	0	159	9	0
7	H	333	0	183	6	0
8	I	102	0	55	3	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
11	I	31	0	11	2	0
All	All	28290	0	28471	390	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 7.

All (390) 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:776:SER:CB	5:F:373:LYS:NZ	2.02	1.23
2:C:769:PRO:HG2	5:F:374:GLY:O	1.40	1.19
2:C:776:SER:HB2	5:F:373:LYS:NZ	1.58	1.19
2:C:769:PRO:CG	5:F:374:GLY:O	1.93	1.17
3:D:233:LYS:NZ	3:D:240:GLU:OE2	1.88	1.04
2:C:776:SER:CB	5:F:373:LYS:HZ3	1.65	1.02
2:C:776:SER:HB2	5:F:373:LYS:HZ3	0.86	1.01
2:C:776:SER:OG	5:F:373:LYS:NZ	1.94	0.97
5:F:392:VAL:CG1	5:F:396:ARG:HB2	2.05	0.86
6:G:16:DG:H8	6:G:16:DG:H5"	1.41	0.85
5:F:368:VAL:HG21	5:F:400:ILE:HG21	1.63	0.80
2:C:774:LEU:HD22	5:F:350:LEU:HD11	1.63	0.79
5:F:392:VAL:HG22	5:F:396:ARG:HD2	1.65	0.79
2:C:776:SER:CB	5:F:373:LYS:HZ2	1.82	0.78
3:D:671:LYS:HE2	5:F:346:THR:HG21	1.66	0.77
3:D:256:GLU:OE1	3:D:274:ARG:NH1	2.19	0.75
5:F:392:VAL:HG13	5:F:396:ARG:HB2	1.69	0.74
5:F:360:LYS:HD3	5:F:411:HIS:ND1	2.02	0.73
3:D:61:GLY:O	3:D:64:LYS:NZ	2.21	0.73
5:F:371:LEU:HD23	5:F:376:ILE:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:776:SER:CB	5:F:373:LYS:CE	2.68	0.72
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.72	0.72
6:G:16:DG:H8	6:G:16:DG:C5'	2.04	0.70
5:F:358:LEU:CD2	5:F:366:ALA:HB1	2.21	0.70
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.73	0.69
5:F:392:VAL:HG11	5:F:396:ARG:HB2	1.74	0.68
5:F:200:LYS:HG3	5:F:201:LYS:HG3	1.76	0.68
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.27	0.68
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.76	0.67
6:G:15:DT:O4	11:I:101:ATP:N6	2.24	0.67
3:D:132:TYR:OH	3:D:568:ARG:NH2	2.28	0.67
2:C:243:ARG:NH2	7:H:9:DG:O6	2.27	0.67
5:F:384:GLU:HG2	5:F:394:ARG:CZ	2.25	0.67
2:C:769:PRO:CG	5:F:374:GLY:C	2.63	0.66
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.77	0.66
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.76	0.66
1:B:88:ARG:NH1	1:B:123:MET:SD	2.68	0.66
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.76	0.66
2:C:793:PRO:HB2	2:C:796:GLU:HG3	1.77	0.66
3:D:704:ARG:NH2	8:I:5:A:O2'	2.29	0.65
2:C:769:PRO:HB2	5:F:375:LEU:HA	1.77	0.65
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.78	0.65
2:C:905:ILE:HG23	2:C:906:PHE:HD1	1.61	0.65
2:C:154:ARG:NH2	2:C:176:VAL:O	2.31	0.64
2:C:769:PRO:HG3	5:F:374:GLY:O	1.91	0.64
3:D:17:LYS:O	3:D:20:SER:OG	2.12	0.64
5:F:358:LEU:HD22	5:F:366:ALA:HB1	1.80	0.64
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.80	0.63
2:C:236:ILE:HG23	2:C:248:PRO:HB2	1.80	0.63
3:D:411:THR:HB	3:D:437:VAL:H	1.62	0.63
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.80	0.62
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.82	0.62
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.81	0.62
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.82	0.62
2:C:614:ARG:NH2	2:C:618:GLY:O	2.32	0.62
2:C:711:GLU:O	2:C:758:ARG:NH1	2.32	0.62
3:D:671:LYS:HE2	5:F:346:THR:CG2	2.30	0.62
5:F:371:LEU:CD2	5:F:376:ILE:HD12	2.30	0.61
3:D:960:LYS:NZ	3:D:1063:GLU:OE1	2.32	0.61
1:A:222:LEU:HD22	1:B:215:VAL:HG23	1.84	0.59
2:C:769:PRO:CB	5:F:375:LEU:HA	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:846:LYS:NZ	8:I:5:A:OP1	2.30	0.59
3:D:136:ASP:OD2	3:D:138:LYS:HE3	2.02	0.59
2:C:640:ARG:NH1	2:C:657:ASP:O	2.35	0.59
5:F:392:VAL:HG22	5:F:396:ARG:CD	2.33	0.59
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.83	0.59
2:C:769:PRO:HB3	5:F:374:GLY:C	2.23	0.58
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.86	0.58
3:D:1468:LEU:HB3	3:D:1470:ARG:HG3	1.86	0.58
2:C:251:ASP:N	2:C:251:ASP:OD1	2.36	0.58
6:G:16:DG:C8	6:G:16:DG:H5"	2.31	0.58
2:C:939:ARG:HB2	2:C:982:PRO:HG3	1.84	0.58
2:C:769:PRO:HA	2:C:772:ARG:HB2	1.84	0.58
3:D:1491:THR:HG21	4:E:89:MET:HG2	1.86	0.58
2:C:846:LYS:HE3	3:D:741:ASP:HB2	1.86	0.58
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.68	0.58
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.86	0.58
2:C:270:GLY:O	2:C:274:ARG:N	2.35	0.58
3:D:241:ILE:HG12	3:D:312:ARG:NH1	2.19	0.57
3:D:431:VAL:HG21	3:D:448:GLU:HG2	1.86	0.57
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.85	0.57
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.86	0.57
3:D:1047:LYS:HD2	3:D:1051:GLU:HG3	1.85	0.57
2:C:595:LEU:HB3	2:C:656:ALA:HB3	1.86	0.57
1:B:84:GLU:OE2	3:D:867:ARG:NH1	2.36	0.57
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.86	0.57
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.85	0.57
5:F:420:ASP:O	5:F:422:LEU:N	2.36	0.57
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.37	0.57
3:D:173:PRO:HA	3:D:209:ARG:HH12	1.70	0.57
7:H:19:DG:H2"	7:H:20:DG:H5'	1.87	0.56
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.87	0.56
5:F:360:LYS:HD3	5:F:411:HIS:CE1	2.39	0.56
3:D:372:ASP:OD1	3:D:372:ASP:N	2.38	0.56
2:C:422:ARG:HG2	7:H:19:DG:OP2	2.06	0.56
5:F:358:LEU:HD23	5:F:366:ALA:HB1	1.86	0.56
1:B:112:ARG:HB3	1:B:125:PRO:HB2	1.88	0.56
5:F:350:LEU:HD13	5:F:421:PHE:CD1	2.41	0.56
5:F:415:THR:HB	5:F:417:LYS:HE3	1.87	0.56
3:D:433:GLY:HA2	3:D:449:SER:H	1.71	0.56
3:D:216:VAL:HG23	3:D:383:GLY:HA2	1.88	0.55
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:THR:HG22	1:B:209:GLU:H	1.71	0.55
2:C:770:GLU:OE1	5:F:351:SER:OG	2.24	0.55
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.87	0.55
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.89	0.55
3:D:573:MET:SD	5:F:210:LEU:HB3	2.46	0.54
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.89	0.54
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.90	0.54
2:C:759:THR:HB	2:C:785:VAL:HB	1.89	0.54
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.41	0.54
2:C:615:TYR:HH	2:C:623:TYR:HH	1.49	0.54
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.88	0.54
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.88	0.54
2:C:769:PRO:CB	5:F:374:GLY:C	2.76	0.54
6:G:16:DG:C8	6:G:16:DG:C5'	2.88	0.54
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.88	0.54
2:C:1052:MET:HG3	3:D:623:VAL:HG11	1.89	0.54
2:C:428:ARG:NH2	2:C:447:ALA:O	2.39	0.54
3:D:504:ASP:OD1	3:D:1388:ARG:NH2	2.41	0.54
5:F:345:ALA:O	5:F:349:LEU:HG	2.07	0.54
1:B:94:LEU:HD21	1:B:97:VAL:HG13	1.90	0.54
5:F:392:VAL:HG12	5:F:397:ILE:HG12	1.90	0.53
2:C:911:GLU:OE2	3:D:1062:ARG:NH1	2.41	0.53
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.90	0.53
2:C:69:LEU:HD12	2:C:97:ARG:HG2	1.90	0.53
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.91	0.53
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.90	0.53
3:D:241:ILE:HG12	3:D:312:ARG:HH12	1.72	0.53
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	1.90	0.53
5:F:164:LYS:HA	5:F:171:LYS:HE3	1.90	0.53
1:B:88:ARG:NH2	1:B:121:GLU:OE1	2.42	0.53
3:D:67:ARG:NH1	5:F:377:ASP:OD1	2.42	0.53
3:D:86:ARG:HB3	3:D:522:PRO:HG2	1.91	0.53
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.91	0.52
3:D:236:TYR:HD2	3:D:322:VAL:HG21	1.74	0.52
3:D:119:SER:HB3	3:D:122:GLU:HG3	1.90	0.52
5:F:396:ARG:HA	5:F:399:GLN:HG2	1.91	0.52
2:C:286:SER:OG	2:C:301:GLU:OE1	2.28	0.52
5:F:404:ALA:O	5:F:408:LEU:HG	2.10	0.52
3:D:520:LEU:O	3:D:525:ARG:NH1	2.43	0.52
2:C:769:PRO:CB	5:F:374:GLY:O	2.56	0.51
3:D:339:TRP:HE1	3:D:341:GLU:HG3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.92	0.51
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.92	0.51
1:A:94:LEU:O	1:A:146:ARG:NH1	2.34	0.51
3:D:486:ARG:HA	3:D:489:ARG:HH21	1.76	0.51
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.93	0.51
2:C:175:GLU:O	2:C:183:SER:OG	2.24	0.51
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.76	0.51
2:C:775:ARG:HG2	2:C:782:ALA:HB2	1.93	0.51
2:C:133:ASP:HB2	2:C:632:ASN:HD21	1.74	0.51
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.44	0.51
1:A:54:THR:HB	1:A:158:ILE:HD12	1.93	0.51
2:C:774:LEU:HD22	5:F:350:LEU:CD1	2.37	0.50
3:D:102:ILE:HD12	3:D:579:ASP:HB3	1.92	0.50
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.75	0.50
2:C:631:SER:HB3	2:C:637:LEU:HG	1.93	0.50
3:D:622:ARG:NH1	6:G:13:DA:OP1	2.43	0.50
2:C:541:SER:OG	2:C:542:VAL:N	2.37	0.50
2:C:578:VAL:HG23	2:C:579:VAL:HG23	1.93	0.50
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.94	0.50
3:D:601:ARG:HD3	5:F:318:GLU:HG2	1.93	0.50
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.94	0.50
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.92	0.50
2:C:16:PRO:HB3	2:C:460:ARG:HH21	1.76	0.49
3:D:710:ARG:HH21	3:D:772:PRO:HG3	1.77	0.49
5:F:265:VAL:O	5:F:269:ASN:ND2	2.31	0.49
1:A:4:SER:O	1:A:189:ARG:NH2	2.45	0.49
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.93	0.49
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.93	0.49
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.94	0.49
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.94	0.49
3:D:500:ARG:HH12	3:D:1390:LEU:HD21	1.77	0.49
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.93	0.49
2:C:160:ALA:HB2	2:C:310:LEU:HD13	1.94	0.49
2:C:397:GLU:N	2:C:633:GLN:OE1	2.42	0.49
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.95	0.49
1:A:44:LEU:HB3	1:A:177:VAL:HG21	1.93	0.49
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.95	0.49
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.78	0.49
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.94	0.48
3:D:675:ARG:NH2	5:F:420:ASP:O	2.46	0.48
2:C:769:PRO:HB3	5:F:375:LEU:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:764:GLU:HB2	3:D:54:LYS:NZ	2.28	0.48
3:D:231:VAL:O	3:D:236:TYR:OH	2.31	0.48
2:C:1001:VAL:HB	3:D:724:GLN:HB2	1.94	0.48
1:A:26:GLU:HB2	1:A:194:LYS:HG3	1.96	0.48
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.94	0.48
3:D:323:GLU:HB2	3:D:334:THR:HB	1.96	0.48
2:C:537:LYS:HD3	2:C:583:LEU:HD11	1.95	0.47
2:C:776:SER:HB3	5:F:373:LYS:CE	2.44	0.47
1:A:124:ASN:N	1:A:124:ASN:OD1	2.47	0.47
3:D:759:ALA:HA	3:D:763:MET:HB2	1.96	0.47
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.48	0.47
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.48	0.47
3:D:899:LEU:HD21	3:D:921:ARG:HD3	1.97	0.47
3:D:539:ASP:OD1	5:F:316:SER:OG	2.26	0.47
2:C:271:GLU:OE1	2:C:274:ARG:NH1	2.47	0.47
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.96	0.47
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.96	0.47
1:A:99:LEU:HB2	1:A:142:VAL:HG23	1.96	0.47
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.96	0.47
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.47	0.47
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.97	0.47
3:D:284:LEU:HD22	3:D:288:MET:HG2	1.97	0.47
2:C:495:THR:OG1	2:C:517:ARG:NE	2.47	0.47
2:C:778:PHE:CD1	5:F:412:GLU:OE2	2.68	0.47
3:D:564:GLU:OE2	5:F:140:ARG:NH2	2.47	0.47
1:B:175:ARG:N	1:B:200:TRP:O	2.43	0.47
5:F:340:SER:HB2	5:F:341:PRO:HD2	1.97	0.47
5:F:357:ALA:O	5:F:361:LEU:HG	2.15	0.47
3:D:1300:SER:OG	3:D:1301:LYS:N	2.48	0.47
1:A:83:LYS:NZ	2:C:698:ASP:OD2	2.48	0.47
3:D:526:PRO:HB2	3:D:528:VAL:HG13	1.97	0.46
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.97	0.46
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.36	0.46
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.98	0.46
3:D:1219:GLU:OE1	4:E:17:TYR:OH	2.24	0.46
3:D:485:SER:O	3:D:487:ALA:N	2.49	0.46
2:C:351:LEU:HD21	2:C:373:VAL:HG13	1.97	0.46
3:D:959:GLU:OE1	3:D:959:GLU:N	2.48	0.46
2:C:637:LEU:HA	2:C:659:PRO:HG3	1.97	0.46
2:C:983:ILE:O	2:C:985:GLY:N	2.42	0.46
1:A:54:THR:HG21	1:A:145:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:680:ASP:H	3:D:943:THR:HB	1.80	0.46
2:C:686:ASP:OD1	2:C:879:ARG:NH1	2.35	0.46
7:H:19:DG:H2''	7:H:20:DG:H2'	1.98	0.46
4:E:47:LYS:HB3	4:E:54:LEU:HG	1.96	0.46
2:C:595:LEU:HD21	2:C:623:TYR:HB3	1.97	0.46
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.97	0.46
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.44	0.46
1:B:32:PHE:HA	1:B:35:THR:HB	1.98	0.46
3:D:233:LYS:HB2	3:D:236:TYR:CZ	2.51	0.45
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.99	0.45
5:F:357:ALA:HB1	5:F:408:LEU:HD22	1.97	0.45
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.98	0.45
5:F:384:GLU:HG2	5:F:394:ARG:NH1	2.31	0.45
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.98	0.45
2:C:884:GLN:O	2:C:888:THR:OG1	2.30	0.45
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.98	0.45
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.98	0.45
2:C:876:VAL:HG11	3:D:949:ILE:HG21	1.98	0.45
3:D:312:ARG:HB3	3:D:312:ARG:HH11	1.81	0.45
3:D:977:ALA:O	3:D:983:LEU:N	2.45	0.45
3:D:7:LYS:NZ	3:D:1458:GLU:OE1	2.49	0.45
5:F:357:ALA:HB1	5:F:408:LEU:CD2	2.47	0.45
2:C:21:ILE:HD12	2:C:455:LEU:HD22	1.97	0.45
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.99	0.45
2:C:769:PRO:HG2	3:D:65:ARG:NH1	2.31	0.45
3:D:131:LYS:HD3	3:D:152:LEU:HB3	1.97	0.45
3:D:661:MET:HG2	3:D:666:ILE:HD12	1.99	0.45
2:C:727:PRO:HB2	2:C:728:HIS:HD2	1.80	0.45
5:F:367:MET:SD	5:F:376:ILE:HD11	2.57	0.45
5:F:340:SER:HB2	5:F:341:PRO:CD	2.47	0.45
2:C:1059:ASP:O	2:C:1063:ARG:N	2.42	0.45
1:B:124:ASN:N	1:B:124:ASN:OD1	2.49	0.45
3:D:804:LEU:H	3:D:827:ILE:HG22	1.82	0.45
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.52	0.44
2:C:502:PRO:HD2	2:C:510:ALA:HB2	1.99	0.44
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.98	0.44
2:C:419:THR:H	2:C:422:ARG:HB2	1.83	0.44
3:D:224:ARG:H	3:D:251:PHE:HE1	1.64	0.44
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.99	0.44
5:F:360:LYS:HB3	5:F:411:HIS:CE1	2.53	0.44
3:D:1089:ALA:HA	6:G:10:DG:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:57:ASP:O	4:E:63:TRP:NE1	2.49	0.44
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.99	0.44
3:D:224:ARG:NH1	3:D:254:GLU:OE2	2.50	0.44
2:C:987:ILE:HD11	3:D:946:GLY:HA2	2.00	0.44
1:A:31:GLY:O	1:A:35:THR:OG1	2.28	0.44
3:D:187:LYS:HB2	3:D:200:ASP:OD2	2.17	0.44
1:A:99:LEU:HD21	1:A:122:ILE:HD11	2.00	0.44
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.90	0.44
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.18	0.43
3:D:1235:GLN:C	3:D:1237:THR:H	2.21	0.43
2:C:230:ARG:HB2	2:C:233:GLU:HG2	2.00	0.43
2:C:673:LEU:HD23	2:C:867:VAL:HA	2.00	0.43
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.53	0.43
2:C:194:VAL:HG22	2:C:221:LEU:HD22	1.99	0.43
3:D:350:HIS:CD2	5:F:232:ARG:HG2	2.53	0.43
1:A:206:THR:HG22	1:A:209:GLU:H	1.83	0.43
2:C:724:ARG:NH2	2:C:734:LEU:O	2.51	0.43
2:C:214:TYR:CD2	2:C:218:VAL:HG23	2.54	0.43
5:F:413:SER:HA	5:F:416:ARG:HG2	2.00	0.43
3:D:1499:ARG:HH12	4:E:81:PRO:HD2	1.83	0.43
2:C:492:ASP:HB3	2:C:518:LYS:HG2	2.00	0.43
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.35	0.43
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	2.00	0.43
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.99	0.43
5:F:201:LYS:HB2	5:F:201:LYS:HE3	1.89	0.43
3:D:1094:LEU:HD22	3:D:1260:ILE:HG12	2.00	0.43
3:D:809:PRO:HB3	3:D:839:LEU:HD13	2.00	0.43
3:D:339:TRP:NE1	3:D:341:GLU:HG3	2.34	0.43
1:A:202:ASP:OD1	1:A:203:GLY:N	2.52	0.43
3:D:1281:VAL:HG22	3:D:1317:ASP:H	1.84	0.43
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.01	0.43
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.00	0.43
2:C:627:ARG:HD3	2:C:638:ASP:OD1	2.19	0.43
2:C:439:CYS:HA	2:C:440:PRO:HD3	1.82	0.43
2:C:938:LYS:HE2	2:C:938:LYS:HB3	1.89	0.43
3:D:693:GLU:HA	4:E:48:MET:HE1	2.01	0.43
2:C:1031:ARG:NH2	3:D:620:GLY:O	2.44	0.43
2:C:474:VAL:HG22	2:C:479:VAL:HG22	2.01	0.43
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.36	0.43
3:D:828:LYS:HG2	3:D:833:GLU:HG2	2.01	0.43
5:F:131:VAL:HG13	5:F:178:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:954:ALA:HB3	3:D:1062:ARG:HG3	1.99	0.42
3:D:827:ILE:HB	3:D:829:VAL:HG23	2.00	0.42
2:C:937:ASP:HB3	2:C:940:GLU:HG3	2.00	0.42
5:F:360:LYS:HD3	5:F:411:HIS:CG	2.54	0.42
3:D:84:ILE:HG13	3:D:88:TYR:HE1	1.84	0.42
3:D:171:LEU:HA	3:D:172:PRO:HD3	1.95	0.42
2:C:144:PRO:HB2	2:C:273:GLY:HA3	2.00	0.42
3:D:260:GLU:HB3	3:D:271:VAL:HB	2.01	0.42
5:F:123:ASP:HA	5:F:124:PRO:HD3	1.91	0.42
2:C:928:LYS:O	2:C:932:GLU:HB2	2.19	0.42
1:B:97:VAL:HG23	1:B:144:VAL:HB	2.01	0.42
3:D:245:LEU:HD22	3:D:249:TYR:HB3	2.01	0.42
3:D:711:LEU:HB3	3:D:714:GLN:HE21	1.85	0.42
2:C:390:GLN:HG3	11:I:101:ATP:H4'	2.02	0.42
3:D:961:LYS:HE3	3:D:961:LYS:HB2	1.91	0.42
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.01	0.42
3:D:714:GLN:HB2	3:D:736:PHE:HZ	1.84	0.42
3:D:214:GLU:HB3	3:D:340:THR:HB	2.00	0.42
3:D:238:PRO:HD3	3:D:318:ARG:HG3	2.02	0.42
3:D:795:VAL:HG12	3:D:876:SER:HB3	2.02	0.42
2:C:810:ASP:HA	2:C:811:PRO:HD3	1.90	0.42
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.52	0.42
2:C:214:TYR:CE2	2:C:311:PHE:HB3	2.54	0.42
3:D:266:GLU:HG3	3:D:314:PRO:HB3	2.02	0.42
1:A:227:ASN:HA	1:A:228:PRO:HD3	1.77	0.42
3:D:273:ARG:HB3	3:D:278:PRO:HA	2.01	0.42
3:D:1205:TYR:CE1	3:D:1366:LYS:HE2	2.55	0.42
3:D:527:MET:SD	3:D:537:THR:HB	2.60	0.42
2:C:261:ILE:HG23	2:C:290:LEU:HB2	2.01	0.42
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.38	0.41
3:D:39:PRO:HG3	3:D:47:GLU:HG3	2.01	0.41
3:D:1102:THR:O	3:D:1222:GLY:HA3	2.20	0.41
3:D:58:CYS:SG	3:D:62:LYS:N	2.92	0.41
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.53	0.41
3:D:87:ARG:HG2	3:D:523:ASP:HB2	2.03	0.41
1:A:199:ILE:HB	1:A:207:PRO:HB3	2.00	0.41
2:C:510:ALA:HB3	2:C:513:VAL:HG12	2.02	0.41
7:H:22:DT:H2"	7:H:23:DG:C8	2.55	0.41
3:D:553:ARG:HH12	5:F:211:ASP:HA	1.84	0.41
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.95	0.41
2:C:122:THR:OG1	2:C:124:ASP:OD1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:14:DG:N2	8:I:2:C:O2	2.52	0.41
3:D:230:TRP:CZ2	3:D:232:GLU:HG2	2.55	0.41
2:C:572:ILE:HG13	2:C:573:ARG:HG2	2.01	0.41
2:C:327:HIS:CE1	2:C:433:THR:HG21	2.55	0.41
2:C:376:ARG:NH2	5:F:279:GLN:OE1	2.54	0.41
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.53	0.41
3:D:48:ARG:NE	3:D:76:CYS:O	2.54	0.41
3:D:896:ALA:O	3:D:900:ILE:HG13	2.21	0.41
1:B:51:THR:OG1	1:B:87:VAL:O	2.23	0.41
5:F:91:VAL:O	5:F:193:ARG:NH2	2.38	0.41
2:C:802:ARG:HB2	2:C:826:TYR:HB2	2.02	0.41
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.02	0.41
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.85	0.41
3:D:321:GLN:HB2	3:D:336:PHE:CD2	2.56	0.41
2:C:1036:GLU:OE2	2:C:1036:GLU:N	2.52	0.41
3:D:272:LEU:HB2	3:D:280:ALA:HB3	2.03	0.41
1:B:18:ARG:NH1	1:B:204:SER:O	2.53	0.41
2:C:657:ASP:OD2	2:C:663:ASN:N	2.50	0.41
2:C:1067:TYR:OH	3:D:674:ARG:NH1	2.54	0.41
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.91	0.41
3:D:750:PRO:O	3:D:756:GLN:NE2	2.54	0.41
3:D:222:GLY:HA2	3:D:333:LEU:O	2.21	0.41
4:E:14:ASP:OD2	4:E:14:ASP:N	2.52	0.41
1:B:77:GLU:HG2	3:D:872:ARG:HH11	1.86	0.41
2:C:543:ASN:OD1	2:C:543:ASN:N	2.53	0.41
3:D:350:HIS:HD2	5:F:232:ARG:HG2	1.85	0.40
6:G:11:DT:H2'	6:G:12:DG:C8	2.56	0.40
3:D:1090:ASP:N	3:D:1090:ASP:OD1	2.54	0.40
5:F:308:LEU:HA	5:F:308:LEU:HD23	1.94	0.40
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.93	0.40
5:F:392:VAL:CG1	5:F:393:THR:N	2.84	0.40
2:C:405:ARG:HH21	2:C:566:THR:HG21	1.85	0.40
3:D:1120:VAL:HA	3:D:1121:PRO:HD3	1.88	0.40
5:F:350:LEU:O	5:F:354:LEU:HG	2.21	0.40
2:C:283:ILE:HD13	2:C:305:PRO:HG2	2.02	0.40
5:F:193:ARG:HB2	7:H:6:DT:H1'	2.02	0.40
3:D:508:ARG:HA	3:D:509:PRO:HD3	1.98	0.40
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.56	0.40
3:D:629:SER:HB3	3:D:726:ILE:HG13	2.03	0.40
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.88	0.40
2:C:501:THR:HA	2:C:502:PRO:HD3	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.57	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	224/315 (71%)	209 (93%)	15 (7%)	0	100	100
1	B	220/315 (70%)	207 (94%)	12 (6%)	1 (0%)	34	76
2	C	1107/1119 (99%)	1029 (93%)	70 (6%)	8 (1%)	26	70
3	D	1480/1524 (97%)	1393 (94%)	77 (5%)	10 (1%)	26	70
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	334/423 (79%)	316 (95%)	16 (5%)	2 (1%)	30	72
All	All	3457/3795 (91%)	3243 (94%)	193 (6%)	21 (1%)	30	72

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	421	PHE
2	C	12	VAL
2	C	211	LEU
3	D	448	GLU
3	D	484	PRO
5	F	361	LEU
2	C	365	ASP
2	C	984	GLU
3	D	320	ALA
3	D	486	ARG
3	D	1440	PHE

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Mol	Chain	Res	Type
1	B	191	ASP
2	C	477	GLY
3	D	530	VAL
2	C	212	GLY
2	C	767	PRO
3	D	665	GLY
3	D	1322	GLY
2	C	769	PRO
3	D	1040	GLY
3	D	668	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	199/273 (73%)	197 (99%)	2 (1%)	82	95
1	B	195/273 (71%)	188 (96%)	7 (4%)	42	79
2	C	936/941 (100%)	908 (97%)	28 (3%)	48	83
3	D	1251/1279 (98%)	1196 (96%)	55 (4%)	35	74
4	E	83/88 (94%)	82 (99%)	1 (1%)	78	94
5	F	294/371 (79%)	282 (96%)	12 (4%)	37	76
All	All	2958/3225 (92%)	2853 (96%)	105 (4%)	43	80

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	VAL
1	A	206	THR
1	B	80	LEU
1	B	94	LEU
1	B	112	ARG
1	B	158	ILE
1	B	186	LEU
1	B	206	THR

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Mol	Chain	Res	Type
1	B	221	HIS
2	C	55	GLU
2	C	81	ASP
2	C	103	LYS
2	C	113	VAL
2	C	141	HIS
2	C	143	SER
2	C	205	GLU
2	C	214	TYR
2	C	251	ASP
2	C	285	LEU
2	C	364	GLU
2	C	434	HIS
2	C	480	THR
2	C	511	GLU
2	C	524	VAL
2	C	539	VAL
2	C	543	ASN
2	C	581	THR
2	C	584	GLU
2	C	610	ARG
2	C	633	GLN
2	C	640	ARG
2	C	657	ASP
2	C	680	ASP
2	C	715	THR
2	C	796	GLU
2	C	939	ARG
2	C	1001	VAL
3	D	32	ILE
3	D	64	LYS
3	D	65	ARG
3	D	106	LYS
3	D	123	LEU
3	D	141	ILE
3	D	198	ARG
3	D	199	LEU
3	D	230	TRP
3	D	256	GLU
3	D	272	LEU
3	D	312	ARG
3	D	331	VAL

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Mol	Chain	Res	Type
3	D	360	ARG
3	D	372	ASP
3	D	415	VAL
3	D	488	ARG
3	D	508	ARG
3	D	525	ARG
3	D	578	VAL
3	D	632	VAL
3	D	709	HIS
3	D	717	GLN
3	D	737	ASN
3	D	754	PHE
3	D	813	LEU
3	D	817	GLU
3	D	847	ASP
3	D	864	VAL
3	D	884	ARG
3	D	894	LYS
3	D	904	VAL
3	D	907	GLU
3	D	940	THR
3	D	974	ILE
3	D	994	GLN
3	D	1011	PHE
3	D	1041	LEU
3	D	1062	ARG
3	D	1090	ASP
3	D	1100	ASP
3	D	1155	VAL
3	D	1188	VAL
3	D	1195	GLN
3	D	1207	TYR
3	D	1235	GLN
3	D	1277	ILE
3	D	1286	THR
3	D	1310	ARG
3	D	1317	ASP
3	D	1464	GLU
3	D	1476	THR
3	D	1482	ARG
3	D	1493	LYS
3	D	1496	GLU

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Mol	Chain	Res	Type
4	E	50	THR
5	F	122	LEU
5	F	141	VAL
5	F	150	THR
5	F	152	ASP
5	F	172	ARG
5	F	209	PHE
5	F	369	LEU
5	F	375	LEU
5	F	382	THR
5	F	383	LEU
5	F	394	ARG
5	F	420	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	565	GLN
2	C	632	ASN
2	C	728	HIS
2	C	969	GLN
2	C	999	HIS
2	C	1026	GLN
2	C	1050	GLN
3	D	294	HIS
3	D	350	HIS
3	D	611	GLN
3	D	714	GLN
3	D	744	GLN
3	D	1124	GLN
3	D	1359	GLN
3	D	1441	GLN
5	F	218	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	4/5 (80%)	0	0

There are no RNA backbone outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
11	ATP	I	101	-	24,33,33	1.67	1 (4%)	31,52,52	1.39	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ATP	I	101	-	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	101	ATP	C5'-C4'	-7.66	1.26	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	I	101	ATP	PA-O3A-PB	-3.71	122.30	132.73
11	I	101	ATP	C5'-C4'-C3'	-3.58	100.98	115.21
11	I	101	ATP	PB-O3B-PG	-3.49	120.97	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	I	101	ATP	2	0

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

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	226/315 (71%)	-0.05	4 (1%) 71 43	76, 116, 149, 155	0
1	B	222/315 (70%)	-0.25	1 (0%) 91 76	63, 90, 119, 133	0
2	C	1111/1119 (99%)	0.07	34 (3%) 52 24	28, 107, 187, 229	0
3	D	1484/1524 (97%)	0.02	36 (2%) 62 32	30, 90, 161, 225	1 (0%)
4	E	94/99 (94%)	-0.04	2 (2%) 67 36	64, 100, 177, 190	0
5	F	338/423 (79%)	0.40	35 (10%) 8 3	94, 135, 226, 265	0
6	G	14/22 (63%)	0.02	0 100 100	78, 106, 188, 200	0
7	H	16/27 (59%)	-0.26	0 100 100	126, 135, 179, 183	0
8	I	5/5 (100%)	-0.63	0 100 100	60, 65, 75, 76	0
All	All	3510/3849 (91%)	0.05	112 (3%) 51 23	28, 104, 177, 265	1 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	391	GLY	8.6
2	C	300	ASP	5.5
5	F	149	GLU	5.1
5	F	392	VAL	4.8
2	C	311	PHE	4.7
5	F	354	LEU	4.7
2	C	367	LEU	4.5
3	D	1299	PHE	4.4
5	F	408	LEU	4.4
2	C	219	GLN	4.3
5	F	358	LEU	4.3
3	D	219	GLU	4.2
2	C	195	LEU	4.0
3	D	268	ALA	4.0
2	C	255	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	207	LEU	3.8
5	F	364	ARG	3.7
5	F	372	ARG	3.7
2	C	64	LEU	3.6
5	F	375	LEU	3.6
3	D	1497	GLU	3.5
3	D	70	GLY	3.4
2	C	224	GLU	3.4
2	C	98	LEU	3.4
2	C	296	GLY	3.3
2	C	251	ASP	3.3
2	C	153	ALA	3.3
5	F	383	LEU	3.2
3	D	409	VAL	3.2
3	D	173	PRO	3.1
3	D	1313	VAL	3.1
3	D	367	ILE	3.0
3	D	321	GLN	3.0
2	C	254	VAL	3.0
5	F	384	GLU	3.0
5	F	357	ALA	2.9
2	C	778	PHE	2.9
5	F	142	ARG	2.9
2	C	107	LEU	2.8
2	C	249	LYS	2.8
3	D	269	PHE	2.8
5	F	394	ARG	2.8
3	D	1298	GLY	2.8
1	A	160	ASP	2.8
2	C	769	PRO	2.8
2	C	304	LEU	2.8
5	F	393	THR	2.8
4	E	89	MET	2.7
1	B	157	GLY	2.7
3	D	63	TYR	2.7
5	F	320	PRO	2.7
2	C	102	HIS	2.7
3	D	379	ALA	2.6
5	F	350	LEU	2.6
3	D	393	ILE	2.6
2	C	159	ILE	2.5
3	D	81	THR	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	280	ALA	2.5
5	F	351	SER	2.5
2	C	223	ASP	2.5
5	F	377	ASP	2.5
3	D	355	VAL	2.5
5	F	410	TYR	2.5
5	F	385	GLU	2.5
3	D	198	ARG	2.4
3	D	1128	VAL	2.4
5	F	143	HIS	2.4
1	A	161	ARG	2.4
3	D	205	TYR	2.4
2	C	814	GLU	2.4
2	C	68	PHE	2.4
2	C	209	ARG	2.3
3	D	305	ALA	2.3
2	C	298	PHE	2.3
4	E	79	LEU	2.3
2	C	372	LEU	2.3
2	C	365	ASP	2.3
5	F	415	THR	2.3
3	D	680	GLN	2.3
5	F	417	LYS	2.3
3	D	282	TYR	2.2
3	D	368	VAL	2.2
3	D	1499	ARG	2.2
3	D	490	ALA	2.2
3	D	1312	LEU	2.2
5	F	367	MET	2.2
5	F	381	HIS	2.2
1	A	94	LEU	2.2
2	C	106	GLY	2.2
3	D	336	PHE	2.2
3	D	183	GLU	2.2
5	F	173	TYR	2.2
2	C	616	GLU	2.1
3	D	345	TYR	2.1
5	F	355	GLU	2.1
5	F	388	ALA	2.1
2	C	811	PRO	2.1
5	F	382	THR	2.1
5	F	369	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	1502	ALA	2.1
3	D	142	LEU	2.1
3	D	276	ASP	2.1
5	F	414	ARG	2.1
3	D	1288	GLU	2.1
2	C	780	GLU	2.1
5	F	148	LYS	2.1
5	F	365	GLU	2.1
2	C	196	LEU	2.0
3	D	485	SER	2.0
1	A	64	GLU	2.0
2	C	222	MET	2.0
5	F	151	LEU	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(\AA^2)	Q<0.9
10	ZN	D	2002	1/1	0.88	0.23	-0.22	238,238,238,238	0
11	ATP	I	101	31/31	0.82	0.24	-0.25	72,98,200,233	0
10	ZN	D	2003	1/1	0.98	0.15	-0.59	47,47,47,47	0
9	MG	D	2001	1/1	0.93	0.10	-1.87	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.