



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:33 AM GMT

PDB ID : 2XGJ
Title : STRUCTURE OF MTR4, A DEXH HELICASE INVOLVED IN NUCLEAR
RNA PROCESSING AND SURVEILLANCE
Authors : Weir, J.R.; Bonneau, F.; Hentschel, J.; Conti, E.
Deposited on : 2010-06-04
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

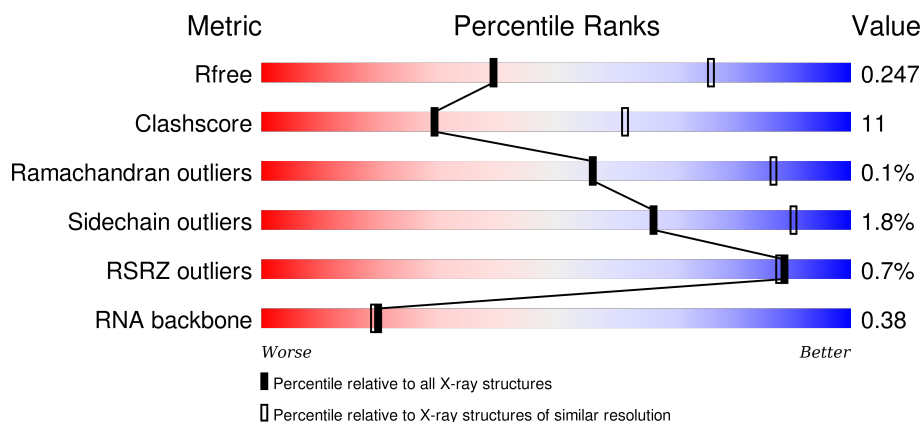
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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	1010	<div> <div style="width: 74%; background-color: green;"></div> <div style="width: 20%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <p>74% 20% • 5%</p>
1	B	1010	<div> <div style="width: 59%; background-color: green;"></div> <div style="width: 18%; background-color: yellow;"></div> <div style="width: 23%; background-color: grey;"></div> </div> <p>59% 18% • 23%</p>
2	C	5	<div> <div style="width: 40%; background-color: green;"></div> <div style="width: 20%; background-color: yellow;"></div> <div style="width: 20%; background-color: orange;"></div> <div style="width: 20%; background-color: red;"></div> </div> <p>40% 20% 20% 20%</p>
2	D	5	<div> <div style="width: 60%; background-color: green;"></div> <div style="width: 40%; background-color: yellow;"></div> </div> <p>60% 40%</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13889 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 ATP-DEPENDENT RNA HELICASE DOB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	964	Total	C	N	O	S	2	0	0
			7513	4796	1280	1394	43			
1	B	777	Total	C	N	O	S	0	0	0
			6024	3866	1012	1108	38			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	HIS	-	EXPRESSION TAG	UNP P47047
A	65	HIS	-	EXPRESSION TAG	UNP P47047
A	66	HIS	-	EXPRESSION TAG	UNP P47047
A	67	HIS	-	EXPRESSION TAG	UNP P47047
A	68	HIS	-	EXPRESSION TAG	UNP P47047
A	69	HIS	-	EXPRESSION TAG	UNP P47047
A	70	GLU	-	EXPRESSION TAG	UNP P47047
A	71	ASN	-	EXPRESSION TAG	UNP P47047
A	72	LEU	-	EXPRESSION TAG	UNP P47047
A	73	TYR	-	EXPRESSION TAG	UNP P47047
A	74	PHE	-	EXPRESSION TAG	UNP P47047
A	75	GLN	-	EXPRESSION TAG	UNP P47047
A	76	GLY	-	EXPRESSION TAG	UNP P47047
A	77	ALA	-	EXPRESSION TAG	UNP P47047
A	78	ALA	-	EXPRESSION TAG	UNP P47047
A	79	SER	-	EXPRESSION TAG	UNP P47047
A	80	MET	-	EXPRESSION TAG	UNP P47047
B	64	HIS	-	EXPRESSION TAG	UNP P47047
B	65	HIS	-	EXPRESSION TAG	UNP P47047
B	66	HIS	-	EXPRESSION TAG	UNP P47047
B	67	HIS	-	EXPRESSION TAG	UNP P47047
B	68	HIS	-	EXPRESSION TAG	UNP P47047
B	69	HIS	-	EXPRESSION TAG	UNP P47047
B	70	GLU	-	EXPRESSION TAG	UNP P47047
B	71	ASN	-	EXPRESSION TAG	UNP P47047

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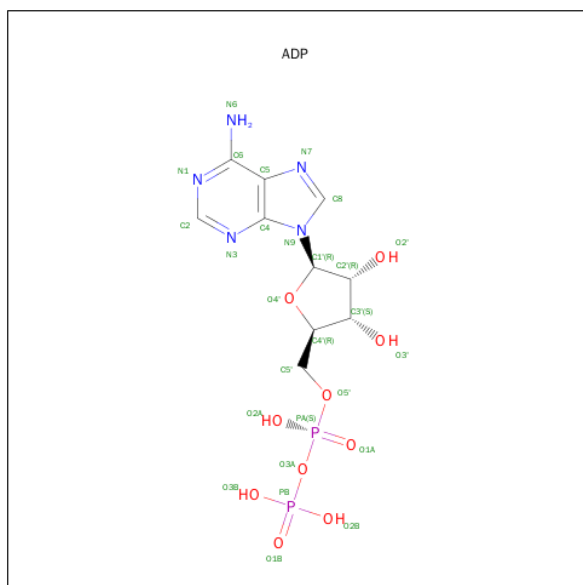
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Chain	Residue	Modelled	Actual	Comment	Reference
B	72	LEU	-	EXPRESSION TAG	UNP P47047
B	73	TYR	-	EXPRESSION TAG	UNP P47047
B	74	PHE	-	EXPRESSION TAG	UNP P47047
B	75	GLN	-	EXPRESSION TAG	UNP P47047
B	76	GLY	-	EXPRESSION TAG	UNP P47047
B	77	ALA	-	EXPRESSION TAG	UNP P47047
B	78	ALA	-	EXPRESSION TAG	UNP P47047
B	79	SER	-	EXPRESSION TAG	UNP P47047
B	80	MET	-	EXPRESSION TAG	UNP P47047

- Molecule 2 is a RNA chain called RNA (5'-(*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total 107	C 50	N 25	O 28	P 4	0	0	0
2	D	5	Total 110	C 50	N 25	O 30	P 5	0	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

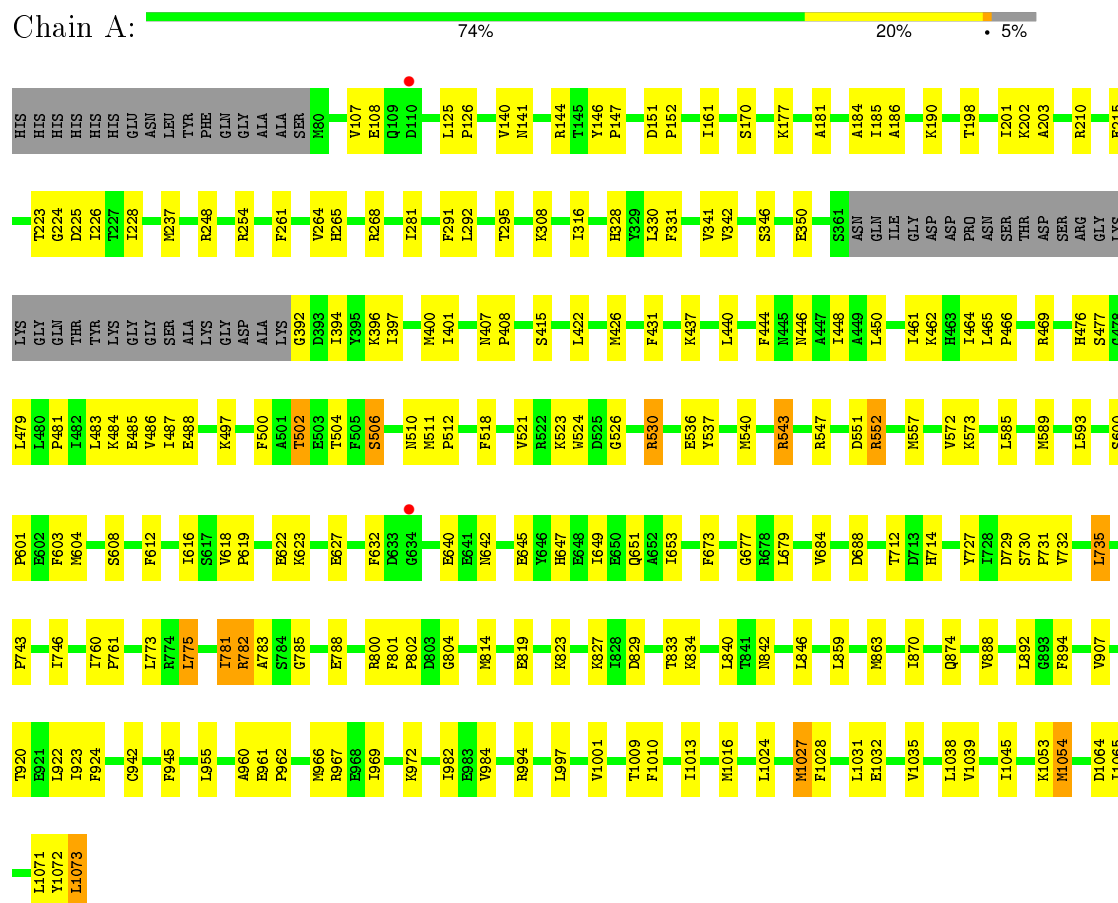
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total 54	O 54	0	0
4	B	27	Total 27	O 27	0	0

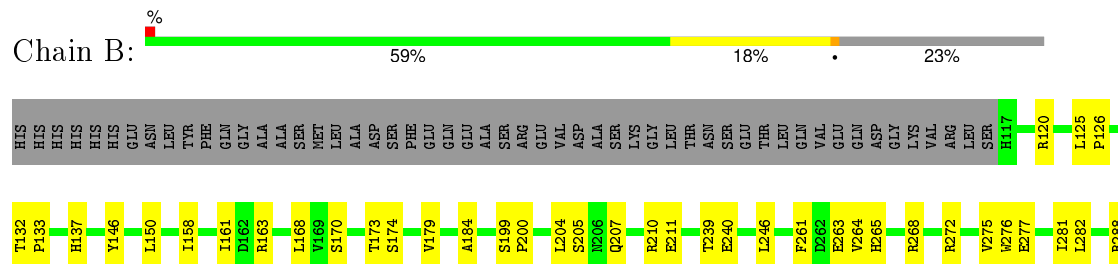
3 Residue-property plots

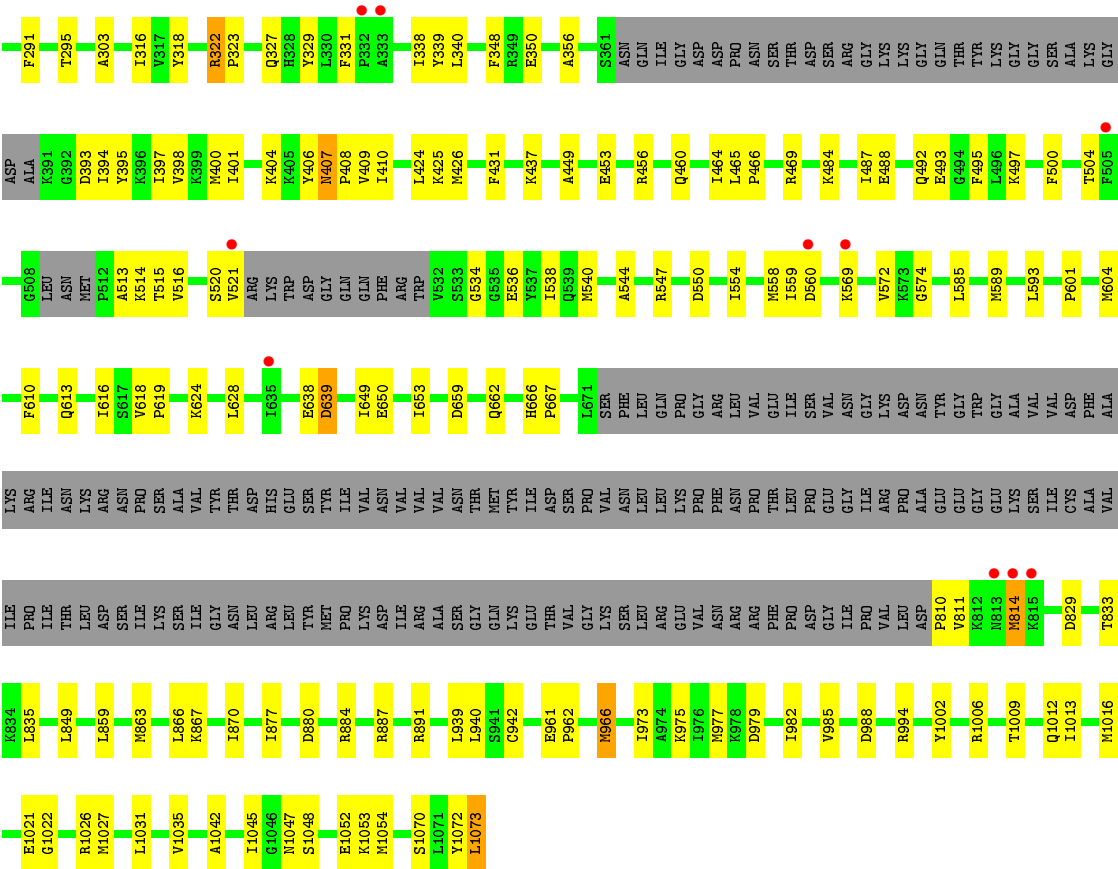
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: ATP-DEPENDENT RNA HELICASE DOB1



• Molecule 1: ATP-DEPENDENT RNA HELICASE DOB1





• Molecule 2: RNA (5'-(*AP*AP*AP*AP*A)-3')



• Molecule 2: RNA (5'-(*AP*AP*AP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.11Å 126.02Å 102.27Å 90.00° 99.21° 90.00°	Depositor
Resolution (Å)	53.45 – 2.90 53.45 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (53.45-2.90) 99.5 (53.45-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.201 , 0.247 0.201 , 0.247	Depositor DCC
R_{free} test set	2806 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.6	EDS
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 55395 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13889	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: ADP

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	0.30	0/7657	0.40	0/10363
1	B	0.23	0/6136	0.38	0/8297
2	C	0.92	0/121	1.65	1/187 (0.5%)
2	D	0.68	0/124	1.22	0/191
All	All	0.29	0/14038	0.44	1/19038 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	A	O4'-C1'-N9	-7.67	102.06	108.20

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	7513	0	7422	162	0
1	B	6024	0	5922	139	0
2	C	107	0	57	12	0
2	D	110	0	56	5	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	54	0	0	0	0
4	B	27	0	0	0	0
All	All	13889	0	13481	309	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 11.

All (309) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ILE:HG21	1:B:409:VAL:HG21	1.46	0.97
1:B:589:MET:HE3	1:B:604:MET:HG2	1.47	0.96
1:B:401:ILE:HG23	1:B:406:TYR:HB2	1.48	0.94
1:A:589:MET:HE3	1:A:604:MET:HG2	1.50	0.93
1:B:409:VAL:HG22	1:B:515:THR:HB	1.49	0.92
2:C:5:A:H5"	2:C:5:A:C8	2.05	0.91
1:B:323:PRO:HB3	1:B:547:ARG:HH11	1.37	0.89
2:C:3:A:H5"	2:C:3:A:H8	1.35	0.88
1:A:859:LEU:O	1:A:863:MET:HG3	1.73	0.88
1:A:511:MET:N	1:A:512:PRO:CD	2.37	0.87
1:A:540:MET:HA	1:A:543:ARG:HE	1.41	0.85
1:A:511:MET:N	1:A:512:PRO:HD2	1.92	0.84
1:A:524:TRP:HD1	1:A:526:GLY:H	1.26	0.84
1:A:504:THR:OG1	2:C:3:A:H4'	1.79	0.83
1:B:322:ARG:HG3	1:B:322:ARG:NH1	1.92	0.83
1:B:323:PRO:HB3	1:B:547:ARG:NH1	1.93	0.81
1:A:552:ARG:CG	1:A:552:ARG:HH11	1.93	0.81
1:A:506:SER:HB3	1:A:543:ARG:HD2	1.62	0.81
2:C:5:A:H5"	2:C:5:A:H8	1.44	0.80
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.43	0.79
1:B:460:GLN:HE21	1:B:1021:GLU:HG2	1.46	0.78
2:C:3:A:C8	2:C:3:A:H5"	2.18	0.77
1:B:264:VAL:HG21	1:B:291:PHE:HB3	1.66	0.77
1:A:407:ASN:HD22	1:A:497:LYS:HD2	1.50	0.76
1:A:248:ARG:HH11	1:A:248:ARG:HG3	1.48	0.76
1:B:460:GLN:NE2	1:B:1021:GLU:HG2	2.01	0.75
1:B:322:ARG:CG	1:B:322:ARG:HH11	2.01	0.74
1:A:679:LEU:HD12	1:A:773:LEU:HB2	1.70	0.74
1:B:401:ILE:HG21	1:B:409:VAL:CG2	2.17	0.74
1:A:407:ASN:ND2	1:A:497:LYS:HD2	2.03	0.73
1:B:327:GLN:HB3	1:B:329:TYR:HE2	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:SER:HA	2:C:2:A:H5'	1.70	0.72
1:A:540:MET:HA	1:A:543:ARG:NE	2.04	0.72
1:A:506:SER:CB	1:A:543:ARG:HD2	2.20	0.71
2:D:2:A:H8	2:D:2:A:H5''	1.56	0.71
1:A:210:ARG:HD3	1:A:1072:TYR:HD1	1.56	0.71
1:B:464:ILE:HD11	1:B:487:ILE:HD11	1.72	0.70
1:A:961:GLU:HB3	1:A:962:PRO:HD3	1.74	0.70
1:A:922:LEU:HD23	1:A:969:ILE:HD12	1.75	0.68
1:A:464:ILE:HD11	1:A:487:ILE:HD11	1.75	0.68
1:B:504:THR:CG2	2:D:3:A:H5''	2.24	0.68
1:B:453:GLU:HA	1:B:456:ARG:HE	1.58	0.67
1:A:223:THR:HG22	1:A:225:ASP:H	1.57	0.67
1:A:510:ASN:C	1:A:512:PRO:HD2	2.14	0.67
1:B:516:VAL:HG23	1:B:544:ALA:HB2	1.76	0.66
1:A:265:HIS:O	1:A:268:ARG:HG2	1.96	0.65
1:B:437:LYS:HB3	1:B:469:ARG:HH21	1.60	0.65
2:C:5:A:H4'	2:C:5:A:OP1	1.94	0.65
1:B:659:ASP:O	1:B:662:GLN:HG2	1.97	0.64
1:A:462:LYS:HE2	1:A:462:LYS:HA	1.79	0.64
1:A:552:ARG:HG2	1:A:552:ARG:HH11	1.62	0.64
1:B:1073:LEU:HD13	1:B:1073:LEU:H	1.61	0.64
1:B:265:HIS:O	1:B:268:ARG:HG2	1.98	0.63
1:B:593:LEU:HD13	1:B:601:PRO:HA	1.81	0.62
1:A:551:ASP:C	1:A:552:ARG:HD3	2.20	0.62
2:D:2:A:C8	2:D:2:A:H5''	2.35	0.61
1:B:1048:SER:O	1:B:1052:GLU:HG2	2.00	0.61
1:B:887:ARG:O	1:B:891:ARG:HG2	2.00	0.61
1:A:645:GLU:O	1:A:649:ILE:HG12	2.01	0.60
1:A:540:MET:HA	1:A:543:ARG:HH21	1.67	0.60
1:B:666:HIS:CG	1:B:667:PRO:HD2	2.37	0.60
1:B:866:LEU:O	1:B:870:ILE:HG23	2.02	0.60
1:A:622:GLU:HG3	1:A:870:ILE:HD13	1.84	0.59
1:B:398:VAL:HG11	1:B:426:MET:HE1	1.83	0.59
1:A:518:PHE:CZ	1:A:540:MET:HB3	2.38	0.58
1:B:961:GLU:HB3	1:B:962:PRO:HD3	1.84	0.58
1:B:348:PHE:CD2	1:B:350:GLU:HG3	2.39	0.58
1:A:346:SER:O	1:A:573:LYS:HD2	2.03	0.58
1:A:552:ARG:HG3	1:A:552:ARG:HH11	1.68	0.58
1:A:775:LEU:HD13	1:A:775:LEU:H	1.68	0.58
1:B:406:TYR:O	1:B:514:LYS:HD3	2.03	0.58
1:B:329:TYR:HD1	1:B:338:ILE:HG22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:PRO:O	1:A:485:GLU:HG2	2.04	0.57
1:B:940:LEU:HD11	1:B:1054:MET:HE1	1.87	0.56
1:B:146:TYR:CZ	1:B:179:VAL:HG13	2.41	0.56
1:B:453:GLU:HG2	1:B:456:ARG:HH21	1.70	0.56
1:A:907:VAL:HG21	1:A:1045:ILE:HD11	1.86	0.56
1:A:161:ILE:HD13	1:A:184:ALA:HB2	1.88	0.56
1:B:407:ASN:HA	1:B:409:VAL:HG23	1.87	0.56
1:A:506:SER:HB3	1:A:543:ARG:CD	2.35	0.55
1:A:248:ARG:HG3	1:A:248:ARG:NH1	2.18	0.55
1:B:547:ARG:HD3	3:B:2074:ADP:O4'	2.06	0.55
1:A:524:TRP:HD1	1:A:526:GLY:N	2.01	0.55
1:B:146:TYR:CE1	1:B:179:VAL:HG13	2.41	0.55
1:B:942:CYS:HA	1:B:994:ARG:O	2.06	0.55
1:B:200:PRO:HG3	1:B:263:GLU:HB2	1.89	0.55
1:B:618:VAL:HB	1:B:619:PRO:HD3	1.88	0.55
1:B:327:GLN:HB3	1:B:329:TYR:CE2	2.38	0.55
1:A:540:MET:HA	1:A:543:ARG:NH2	2.22	0.55
1:A:732:VAL:O	1:A:735:LEU:HD13	2.07	0.55
1:A:955:LEU:HB2	1:A:960:ALA:HB2	1.88	0.54
1:A:540:MET:HG2	1:A:543:ARG:HH21	1.73	0.54
1:B:593:LEU:HD21	1:B:604:MET:HE2	1.89	0.54
1:A:870:ILE:O	1:A:874:GLN:HG2	2.08	0.54
1:B:534:GLY:HA3	1:B:574:GLY:HA3	1.89	0.54
1:A:484:LYS:O	1:A:488:GLU:HG3	2.09	0.53
1:A:254:ARG:NH1	1:A:254:ARG:HB2	2.22	0.53
1:A:585:LEU:HD23	1:A:589:MET:HE1	1.90	0.53
1:A:735:LEU:O	1:A:735:LEU:HD22	2.08	0.53
1:B:426:MET:HG3	1:B:500:PHE:CZ	2.44	0.53
1:B:939:LEU:HD11	1:B:966:MET:HG2	1.90	0.53
1:B:200:PRO:HD2	1:B:204:LEU:HD23	1.90	0.53
1:A:727:TYR:CE2	1:A:729:ASP:HB2	2.44	0.53
1:B:1002:TYR:CE2	1:B:1006:ARG:HD2	2.44	0.52
1:A:552:ARG:HD3	1:A:552:ARG:N	2.24	0.52
1:B:493:GLU:HB3	1:B:495:PHE:CD2	2.45	0.52
1:B:973:ILE:O	1:B:977:MET:HG3	2.09	0.52
1:B:1070:SER:HB3	1:B:1073:LEU:HD21	1.91	0.51
1:A:107:VAL:HG22	1:A:108:GLU:H	1.74	0.51
1:A:942:CYS:HA	1:A:994:ARG:O	2.10	0.51
1:B:484:LYS:O	1:B:488:GLU:HG3	2.11	0.51
1:A:1013:ILE:HA	1:A:1016:MET:HE2	1.93	0.51
1:A:540:MET:HG2	1:A:543:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:PHE:HB3	1:A:497:LYS:HG3	1.93	0.51
1:B:394:ILE:HD12	1:B:394:ILE:H	1.76	0.51
1:B:520:SER:O	1:B:521:VAL:C	2.48	0.51
1:A:593:LEU:HD13	1:A:601:PRO:HA	1.91	0.50
1:A:107:VAL:HG22	1:A:108:GLU:N	2.27	0.50
1:A:712:THR:HG22	1:A:714:HIS:H	1.76	0.50
1:A:647:HIS:O	1:A:651:GLN:HG2	2.11	0.50
1:B:1042:ALA:HA	1:B:1045:ILE:HG22	1.93	0.50
1:B:210:ARG:HD2	1:B:1072:TYR:HD1	1.77	0.50
1:B:585:LEU:HD23	1:B:589:MET:HE1	1.94	0.50
1:A:261:PHE:HB3	1:A:264:VAL:HG22	1.92	0.50
1:B:1073:LEU:HD13	1:B:1073:LEU:N	2.26	0.50
1:A:330:LEU:HD12	1:A:341:VAL:HG11	1.93	0.50
1:B:173:THR:O	1:B:174:SER:HB2	2.11	0.49
1:A:923:ILE:HD11	1:A:1038:LEU:HD22	1.94	0.49
1:A:342:VAL:HG21	1:A:572:VAL:HG12	1.95	0.49
1:A:1064:ASP:CG	1:A:1065:ILE:H	2.15	0.49
1:A:552:ARG:NH1	1:A:552:ARG:HG2	2.22	0.49
1:A:537:TYR:HA	1:A:540:MET:HB2	1.94	0.49
1:B:397:ILE:O	1:B:401:ILE:HG13	2.13	0.49
1:B:401:ILE:HG23	1:B:406:TYR:CB	2.31	0.48
1:B:398:VAL:HG11	1:B:426:MET:CE	2.42	0.48
1:B:1009:THR:HB	1:B:1012:GLN:HG3	1.95	0.48
1:B:329:TYR:CZ	1:B:340:LEU:HD12	2.49	0.48
1:B:624:LYS:O	1:B:628:LEU:HG	2.13	0.48
1:A:1024:LEU:O	1:A:1027:MET:HG3	2.14	0.48
1:A:407:ASN:HB2	1:A:408:PRO:HA	1.95	0.48
1:B:170:SER:OG	1:B:295:THR:HA	2.14	0.48
1:A:540:MET:HA	1:A:543:ARG:CZ	2.42	0.48
1:B:303:ALA:HB2	1:B:316:ILE:CG2	2.44	0.48
1:A:618:VAL:HB	1:A:619:PRO:HD3	1.96	0.48
1:A:540:MET:CA	1:A:543:ARG:HE	2.18	0.48
1:B:348:PHE:HD2	1:B:350:GLU:HG3	1.79	0.48
1:A:773:LEU:HD11	1:A:801:PHE:CE2	2.49	0.48
1:B:1022:GLY:O	1:B:1026:ARG:HG3	2.13	0.48
1:B:536:GLU:O	1:B:540:MET:HG3	2.13	0.48
1:B:410:ILE:HG13	1:B:513:ALA:HB2	1.96	0.48
1:B:239:THR:HG22	1:B:275:VAL:HG12	1.95	0.48
1:B:261:PHE:HB3	1:B:264:VAL:HG22	1.96	0.47
1:B:628:LEU:HD12	1:B:866:LEU:HD12	1.97	0.47
1:A:479:LEU:O	1:A:484:LYS:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:TYR:CG	1:B:356:ALA:HB2	2.49	0.47
1:B:504:THR:HG23	2:D:3:A:H5"	1.96	0.47
1:B:161:ILE:HD13	1:B:184:ALA:HB2	1.95	0.47
1:A:254:ARG:HH11	1:A:254:ARG:HB2	1.79	0.47
1:B:638:GLU:O	1:B:639:ASP:CB	2.63	0.47
1:B:199:SER:HB2	1:B:205:SER:OG	2.14	0.47
1:A:888:VAL:O	1:A:892:LEU:HD23	2.15	0.47
1:B:426:MET:HG3	1:B:500:PHE:HZ	1.79	0.47
1:B:453:GLU:HA	1:B:456:ARG:NE	2.28	0.47
1:B:393:ASP:O	1:B:397:ILE:HG13	2.15	0.46
1:A:523:LYS:HD3	1:A:530:ARG:HH21	1.79	0.46
1:A:945:PHE:HD2	1:A:994:ARG:HB2	1.79	0.46
1:A:552:ARG:CG	1:A:552:ARG:NH1	2.62	0.46
1:A:1031:LEU:O	1:A:1035:VAL:HG23	2.15	0.46
1:A:223:THR:HG22	1:A:224:GLY:N	2.29	0.46
1:A:316:ILE:HG13	1:A:316:ILE:O	2.15	0.46
1:A:394:ILE:HD12	1:A:394:ILE:H	1.80	0.46
1:A:437:LYS:HE3	1:A:469:ARG:HB3	1.97	0.46
1:A:612:PHE:O	1:A:616:ILE:HG12	2.15	0.46
1:B:985:VAL:HB	1:B:988:ASP:HB2	1.98	0.46
1:A:400:MET:CE	1:A:401:ILE:HG13	2.45	0.46
1:A:781:ILE:HG13	1:A:782:ARG:N	2.30	0.46
1:B:207:GLN:O	1:B:211:GLU:HG2	2.15	0.46
1:A:823:LYS:O	1:A:827:LYS:HG3	2.16	0.46
1:A:502:THR:HG21	2:C:3:A:P	2.55	0.46
1:B:137:HIS:CE1	1:B:163:ARG:HG3	2.50	0.46
1:A:201:ILE:HG22	1:A:203:ALA:H	1.81	0.46
1:A:892:LEU:HB3	1:A:894:PHE:CE1	2.51	0.46
1:B:120:ARG:HB3	1:B:318:TYR:HB3	1.97	0.46
1:A:760:ILE:HA	1:A:761:PRO:HD3	1.81	0.45
1:A:801:PHE:HB3	1:A:804:GLY:O	2.15	0.45
1:B:331:PHE:CD2	1:B:558:MET:HG2	2.51	0.45
1:B:464:ILE:CD1	1:B:487:ILE:HD11	2.44	0.45
1:A:210:ARG:HD3	1:A:1072:TYR:CD1	2.43	0.45
1:B:666:HIS:ND1	1:B:667:PRO:HD2	2.30	0.45
1:A:264:VAL:HG21	1:A:291:PHE:HB3	1.97	0.45
1:A:536:GLU:O	1:A:540:MET:HG3	2.16	0.45
1:A:485:GLU:HB3	1:A:1072:TYR:HE2	1.82	0.45
1:A:331:PHE:CD2	1:A:397:ILE:HD11	2.50	0.45
1:A:448:ILE:HD12	1:A:461:ILE:HD13	1.97	0.45
1:B:613:GLN:O	1:B:616:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:C	1:A:440:LEU:HD23	2.37	0.45
1:B:1045:ILE:HG23	1:B:1047:ASN:H	1.82	0.45
1:B:810:PRO:O	1:B:814:MET:HG3	2.16	0.45
1:A:649:ILE:O	1:A:653:ILE:HG13	2.16	0.45
1:A:781:ILE:HD11	1:A:783:ALA:HB2	1.98	0.45
1:A:198:THR:HA	1:A:237:MET:O	2.17	0.45
1:B:465:LEU:HB3	1:B:466:PRO:HD3	1.99	0.44
1:A:151:ASP:CG	1:A:152:PRO:HD2	2.37	0.44
1:A:177:LYS:HB3	1:A:292:LEU:HD22	1.99	0.44
1:A:422:LEU:O	1:A:426:MET:HG2	2.17	0.44
1:B:504:THR:HG22	2:D:3:A:H5''	1.98	0.44
1:A:223:THR:CG2	1:A:224:GLY:N	2.79	0.44
1:A:521:VAL:HG12	1:A:521:VAL:O	2.17	0.44
1:B:515:THR:HG23	1:B:554:ILE:HB	1.99	0.44
2:C:3:A:C8	2:C:3:A:C5'	2.97	0.44
1:A:540:MET:CG	1:A:543:ARG:HH21	2.31	0.44
1:A:392:GLY:O	1:A:396:LYS:HG3	2.18	0.44
1:A:125:LEU:HA	1:A:126:PRO:HD3	1.89	0.44
1:B:150:LEU:HD13	1:B:158:ILE:HD12	2.00	0.44
1:B:488:GLU:O	1:B:492:GLN:HG3	2.17	0.44
1:A:730:SER:HA	1:A:731:PRO:HD3	1.77	0.44
1:B:240:GLU:OE2	1:B:272:ARG:HD2	2.17	0.44
1:A:511:MET:H	1:A:512:PRO:CD	2.28	0.44
1:A:485:GLU:HG3	1:A:1071:LEU:HD12	2.00	0.43
1:A:684:VAL:CG1	1:A:688:ASP:HB2	2.48	0.43
1:A:677:GLY:O	1:A:775:LEU:HD13	2.17	0.43
1:B:210:ARG:HD2	1:B:1072:TYR:CD1	2.53	0.43
1:A:537:TYR:HA	1:A:540:MET:SD	2.57	0.43
1:B:867:LYS:HA	1:B:870:ILE:HG12	1.99	0.43
1:B:538:ILE:HD11	1:B:574:GLY:O	2.18	0.43
1:A:186:ALA:O	1:A:190:LYS:HG3	2.18	0.43
1:A:144:ARG:HH22	1:A:215:GLU:CG	2.31	0.43
1:B:460:GLN:OE1	1:B:460:GLN:N	2.39	0.43
1:B:424:LEU:C	1:B:426:MET:H	2.22	0.43
1:A:1009:THR:HG22	1:A:1010:PHE:N	2.34	0.43
1:B:1053:LYS:HE3	1:B:1053:LYS:HB2	1.85	0.43
1:A:834:LYS:HB2	1:A:834:LYS:HE3	1.77	0.43
1:A:477:SER:HA	1:A:484:LYS:NZ	2.34	0.43
1:B:329:TYR:CD1	1:B:338:ILE:HG22	2.51	0.43
1:B:348:PHE:CD1	1:B:569:LYS:HG2	2.54	0.43
1:B:977:MET:O	1:B:982:ILE:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ASN:HB2	1:B:408:PRO:HA	2.01	0.43
1:B:410:ILE:HG13	1:B:513:ALA:CB	2.49	0.42
1:A:146:TYR:HA	1:A:147:PRO:HD3	1.92	0.42
1:A:623:LYS:O	1:A:627:GLU:HG3	2.18	0.42
1:A:523:LYS:HG2	1:A:524:TRP:N	2.34	0.42
1:B:331:PHE:O	1:B:331:PHE:CD2	2.72	0.42
1:A:281:ILE:HD11	1:A:608:SER:HA	2.01	0.42
1:A:202:LYS:NZ	2:C:5:A:H3'	2.34	0.42
1:B:649:ILE:O	1:B:653:ILE:HG13	2.20	0.42
1:A:640:GLU:HG2	1:A:642:ASN:H	1.84	0.42
1:A:1028:PHE:O	1:A:1032:GLU:HG3	2.19	0.42
1:B:407:ASN:HD22	1:B:407:ASN:N	2.17	0.42
1:A:444:PHE:O	1:A:448:ILE:HG12	2.20	0.42
1:B:395:TYR:CD2	1:B:395:TYR:C	2.93	0.42
1:B:975:LYS:HE2	1:B:979:ASP:OD1	2.20	0.42
1:A:800:ARG:C	1:A:802:PRO:HD3	2.40	0.42
1:B:650:GLU:OE1	1:B:835:LEU:HD21	2.20	0.42
1:B:125:LEU:HA	1:B:126:PRO:HD3	1.87	0.42
1:A:524:TRP:CD1	1:A:526:GLY:N	2.80	0.42
1:A:743:PRO:HD2	1:A:746:ILE:HD12	2.02	0.42
1:A:1053:LYS:HB2	1:A:1053:LYS:HE3	1.92	0.42
1:A:632:PHE:HD2	1:A:859:LEU:HB2	1.85	0.42
1:A:521:VAL:HG22	1:A:557:MET:HG2	2.01	0.42
1:A:226:ILE:HG22	1:A:228:ILE:HG13	2.02	0.42
1:A:819:GLU:O	1:A:823:LYS:HG3	2.19	0.41
1:A:785:GLY:HA2	1:A:788:GLU:OE1	2.20	0.41
1:A:140:VAL:HG23	1:A:141:ASN:N	2.34	0.41
1:A:476:HIS:HB2	2:C:3:A:OP1	2.20	0.41
1:B:329:TYR:HB3	1:B:338:ILE:HG22	2.01	0.41
1:B:639:ASP:CB	1:B:849:LEU:HD13	2.50	0.41
1:A:181:ALA:O	1:A:185:ILE:HG13	2.20	0.41
1:A:673:PHE:CZ	1:A:814:MET:HA	2.55	0.41
1:B:200:PRO:HA	1:B:276:TRP:CZ2	2.55	0.41
1:B:810:PRO:HB2	1:B:811:VAL:H	1.48	0.41
1:A:600:SER:O	1:A:603:PHE:HB3	2.19	0.41
1:B:465:LEU:O	1:B:469:ARG:HG3	2.20	0.41
1:A:446:ASN:O	1:A:450:LEU:HD13	2.21	0.41
1:A:483:LEU:HA	1:A:486:VAL:HG12	2.02	0.41
1:B:431:PHE:CB	1:B:497:LYS:HG3	2.50	0.41
1:A:840:LEU:O	1:A:846:LEU:HD22	2.21	0.41
1:B:400:MET:O	1:B:404:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1002:TYR:O	1:B:1006:ARG:HG3	2.21	0.41
1:B:431:PHE:HB3	1:B:497:LYS:HG3	2.03	0.41
1:B:559:ILE:HD12	1:B:560:ASP:H	1.86	0.41
1:A:982:ILE:HG22	1:A:984:VAL:HG23	2.03	0.41
1:B:246:LEU:HD13	1:B:282:LEU:HB2	2.02	0.41
1:A:426:MET:HG3	1:A:500:PHE:CZ	2.56	0.41
1:B:277:GLU:O	1:B:281:ILE:HG13	2.21	0.41
1:A:1073:LEU:HG	1:A:1073:LEU:H	1.71	0.41
1:B:168:LEU:HD13	1:B:291:PHE:HB2	2.03	0.41
1:A:485:GLU:H	1:A:485:GLU:HG2	1.63	0.41
1:B:395:TYR:HD1	1:B:425:LYS:O	2.04	0.41
1:B:572:VAL:HG12	1:B:572:VAL:O	2.21	0.41
1:B:829:ASP:O	1:B:833:THR:HG23	2.21	0.41
1:A:537:TYR:O	1:A:540:MET:HB2	2.21	0.41
1:B:859:LEU:O	1:B:863:MET:HG3	2.21	0.41
1:B:132:THR:O	1:B:133:PRO:C	2.59	0.41
1:A:170:SER:OG	1:A:295:THR:HA	2.21	0.41
1:A:997:LEU:O	1:A:1001:VAL:HG23	2.20	0.40
1:A:476:HIS:O	1:A:484:LYS:HE2	2.21	0.40
1:A:506:SER:HB3	1:A:543:ARG:CZ	2.51	0.40
1:A:1039:VAL:HG22	1:A:1054:MET:HB3	2.04	0.40
1:B:880:ASP:O	1:B:884:ARG:HG3	2.21	0.40
1:B:610:PHE:HD2	1:B:877:ILE:HD13	1.86	0.40
1:A:465:LEU:N	1:A:466:PRO:CD	2.84	0.40
1:B:1013:ILE:HA	1:B:1016:MET:CE	2.51	0.40
1:A:202:LYS:HZ2	2:C:5:A:H3'	1.85	0.40
1:B:449:ALA:HA	1:B:456:ARG:HH11	1.86	0.40
1:A:328:HIS:HB2	1:A:342:VAL:HB	2.03	0.40
1:A:684:VAL:HG13	1:A:688:ASP:HB2	2.03	0.40
1:A:829:ASP:O	1:A:833:THR:HG23	2.22	0.40
1:A:920:THR:O	1:A:924:PHE:HD2	2.05	0.40
1:B:1031:LEU:O	1:B:1035:VAL:HG23	2.21	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	960/1010 (95%)	934 (97%)	25 (3%)	1 (0%)	56	87
1	B	767/1010 (76%)	728 (95%)	38 (5%)	1 (0%)	56	87
All	All	1727/2020 (86%)	1662 (96%)	63 (4%)	2 (0%)	56	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	781	ILE
1	B	639	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	797/891 (90%)	779 (98%)	18 (2%)	58	87
1	B	627/891 (70%)	619 (99%)	8 (1%)	76	94
All	All	1424/1782 (80%)	1398 (98%)	26 (2%)	66	90

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	LYS
1	A	350	GLU
1	A	502	THR
1	A	506	SER
1	A	530	ARG
1	A	543	ARG
1	A	547	ARG
1	A	552	ARG
1	A	735	LEU
1	A	775	LEU

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Mol	Chain	Res	Type
1	A	782	ARG
1	A	842	ASN
1	A	966	MET
1	A	967	ARG
1	A	972	LYS
1	A	1027	MET
1	A	1054	MET
1	A	1073	LEU
1	B	288	ARG
1	B	322	ARG
1	B	407	ASN
1	B	550	ASP
1	B	814	MET
1	B	966	MET
1	B	1027	MET
1	B	1073	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	4/5 (80%)	2 (50%)	0
2	D	4/5 (80%)	0	0
All	All	8/10 (80%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	3	A
2	C	5	A

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	2074	-	22,29,29	1.01	1 (4%)	27,45,45	1.86	4 (14%)
3	ADP	B	2074	-	22,29,29	1.00	1 (4%)	27,45,45	1.87	3 (11%)

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
3	ADP	A	2074	-	-	0/12/32/32	0/3/3/3
3	ADP	B	2074	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2074	ADP	C5-C4	3.09	1.47	1.40
3	A	2074	ADP	C5-C4	3.11	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2074	ADP	N3-C2-N1	-6.74	123.73	128.89
3	A	2074	ADP	N3-C2-N1	-6.73	123.74	128.89
3	B	2074	ADP	PA-O3A-PB	-3.84	119.80	132.67
3	A	2074	ADP	PA-O3A-PB	-3.45	121.09	132.67
3	A	2074	ADP	C4-C5-N7	-3.25	106.49	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2074	ADP	C4-C5-N7	-3.23	106.51	109.48
3	A	2074	ADP	C2'-C1'-N9	-2.11	111.06	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2074	ADP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	964/1010 (95%)	-0.32	2 (0%) 95 95	19, 44, 83, 111	12 (1%)
1	B	777/1010 (76%)	-0.26	10 (1%) 79 78	25, 54, 94, 117	1 (0%)
2	C	5/5 (100%)	0.24	0 100 100	52, 53, 73, 77	0
2	D	5/5 (100%)	0.04	0 100 100	66, 72, 75, 109	0
All	All	1751/2030 (86%)	-0.29	12 (0%) 89 88	19, 49, 89, 117	13 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	634	GLY	2.8
1	B	505	PHE	2.7
1	B	333	ALA	2.6
1	B	635	ILE	2.6
1	A	110	ASP	2.5
1	B	815	LYS	2.4
1	B	569	LYS	2.3
1	B	521	VAL	2.2
1	B	560	ASP	2.1
1	B	813	ASN	2.1
1	B	332	PRO	2.1
1	B	814	MET	2.0

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

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

6.3 Carbohydrates ⓘ

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
3	ADP	A	2074	27/27	0.96	0.14	-1.12	33,45,61,69	0
3	ADP	B	2074	27/27	0.96	0.13	-1.14	51,63,75,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.