



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 01:57 AM EST

PDB ID : 1FW6
Title : CRYSTAL STRUCTURE OF A TAQ MUTS-DNA-ADP TERNARY COMPLEX
Authors : Junop, M.S.; Obmolova, G.; Rausch, K.; Hsieh, P.; Yang, W.
Deposited on : 2000-09-21
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

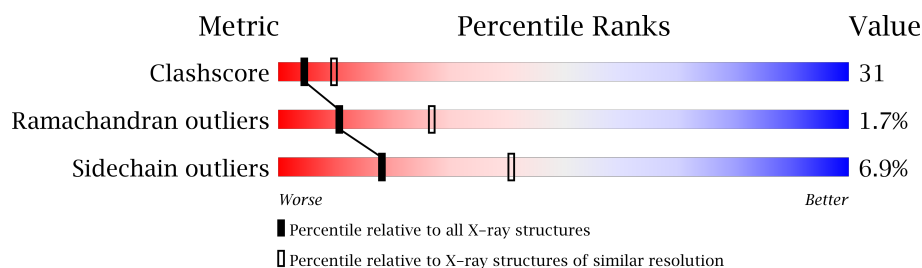
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	23	
2	D	22	
3	A	768	
3	B	768	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13165 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 DNA chain called 5'-D(*GP*CP*GP*AP*CP*GP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*CP*TP*CP*GP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	23	Total	C	N	O	P	0	0	0
			469	222	87	138	22			

- Molecule 2 is a DNA chain called 5'-D(*GP*GP*AP*CP*GP*AP*GP*CP*CP*GP*CP*C*P*GP*CP*TP*AP*GP*CP*GP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	22	Total	C	N	O	P	0	0	0
			450	212	88	129	21			

- Molecule 3 is a protein called DNA MISMATCH REPAIR PROTEIN MUTS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	759	Total	C	N	O	S	Se	0	0	0
			6006	3825	1068	1099	1	13			
3	B	749	Total	C	N	O	S	Se	0	0	0
			5936	3784	1055	1083	1	13			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	4	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	70	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	88	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	201	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	250	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	481	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	574	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	586	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	640	MSE	MET	MODIFIED RESIDUE	UNP Q56215

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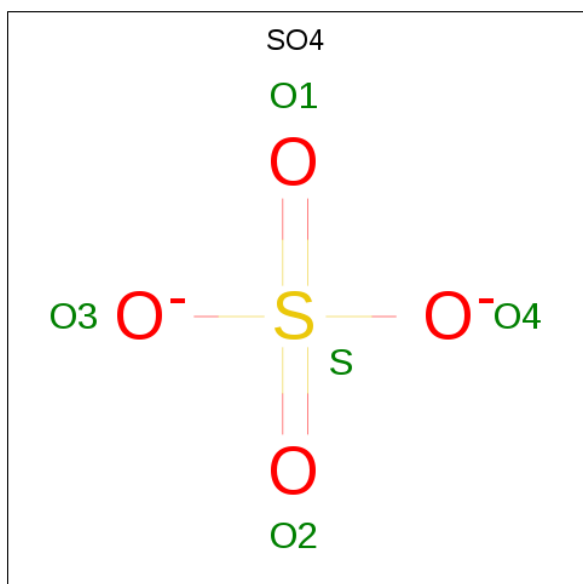
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Chain	Residue	Modelled	Actual	Comment	Reference
A	643	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	744	MSE	MET	MODIFIED RESIDUE	UNP Q56215
A	762	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1001	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1004	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1070	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1088	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1201	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1250	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1481	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1574	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1586	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1640	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1643	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1744	MSE	MET	MODIFIED RESIDUE	UNP Q56215
B	1762	MSE	MET	MODIFIED RESIDUE	UNP Q56215

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

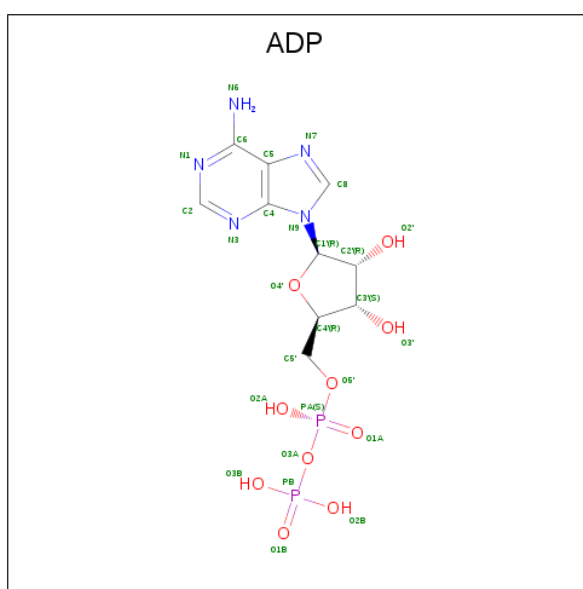
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	4	Total O 4 4	0	0
7	D	4	Total O 4 4	0	0
7	A	105	Total O 105 105	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	115	Total	O	0	0
			115	115		

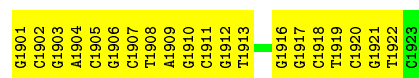
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

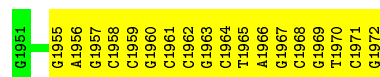
- Molecule 1: 5'-D(*GP*CP*GP*AP*CP*GP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*CP*TP*CP*GP*TP*C)-3'

Chain C: 



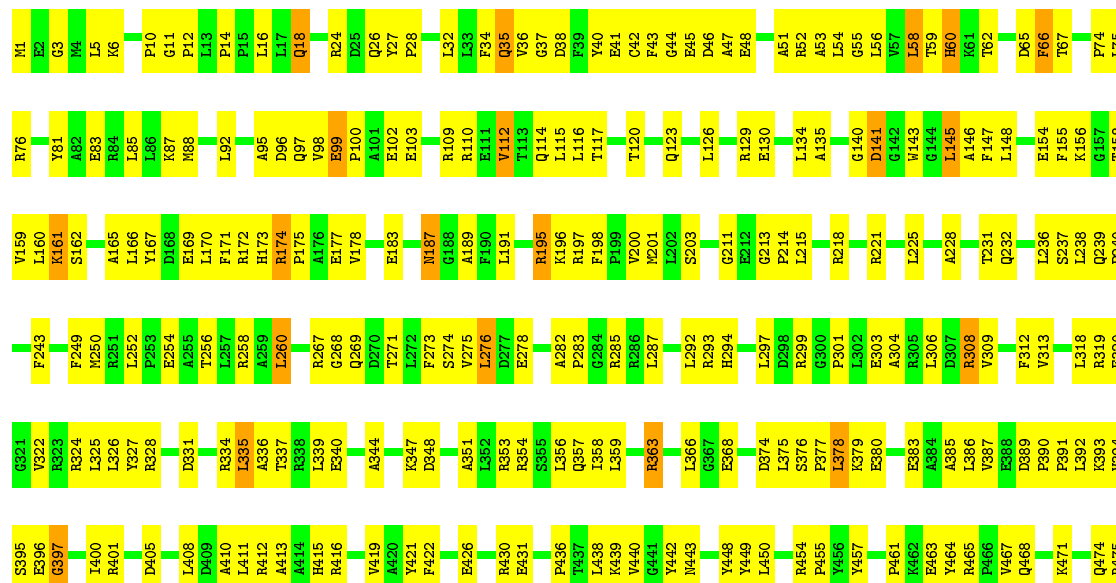
- Molecule 2: 5'-D(*GP*GP*AP*CP*GP*AP*GP*CP*CP*GP*CP*CP*GP*CP*TP*AP*GP*CP*GP*TP*CP*G)-3'

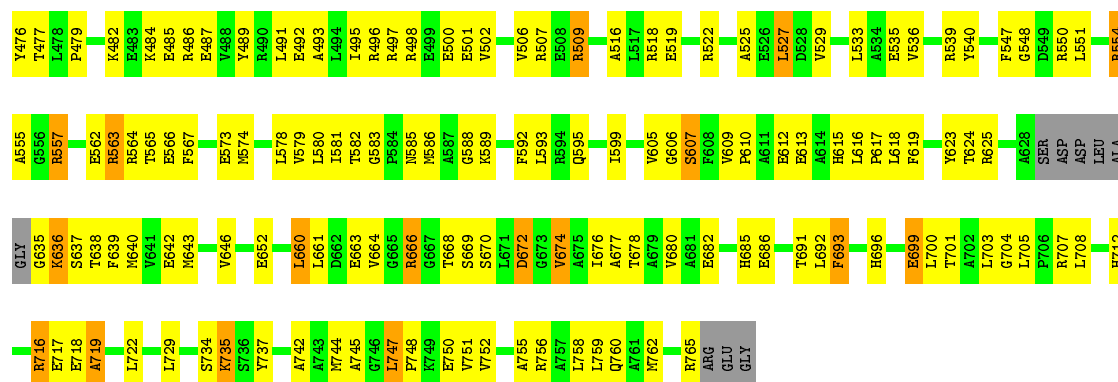
Chain D: 



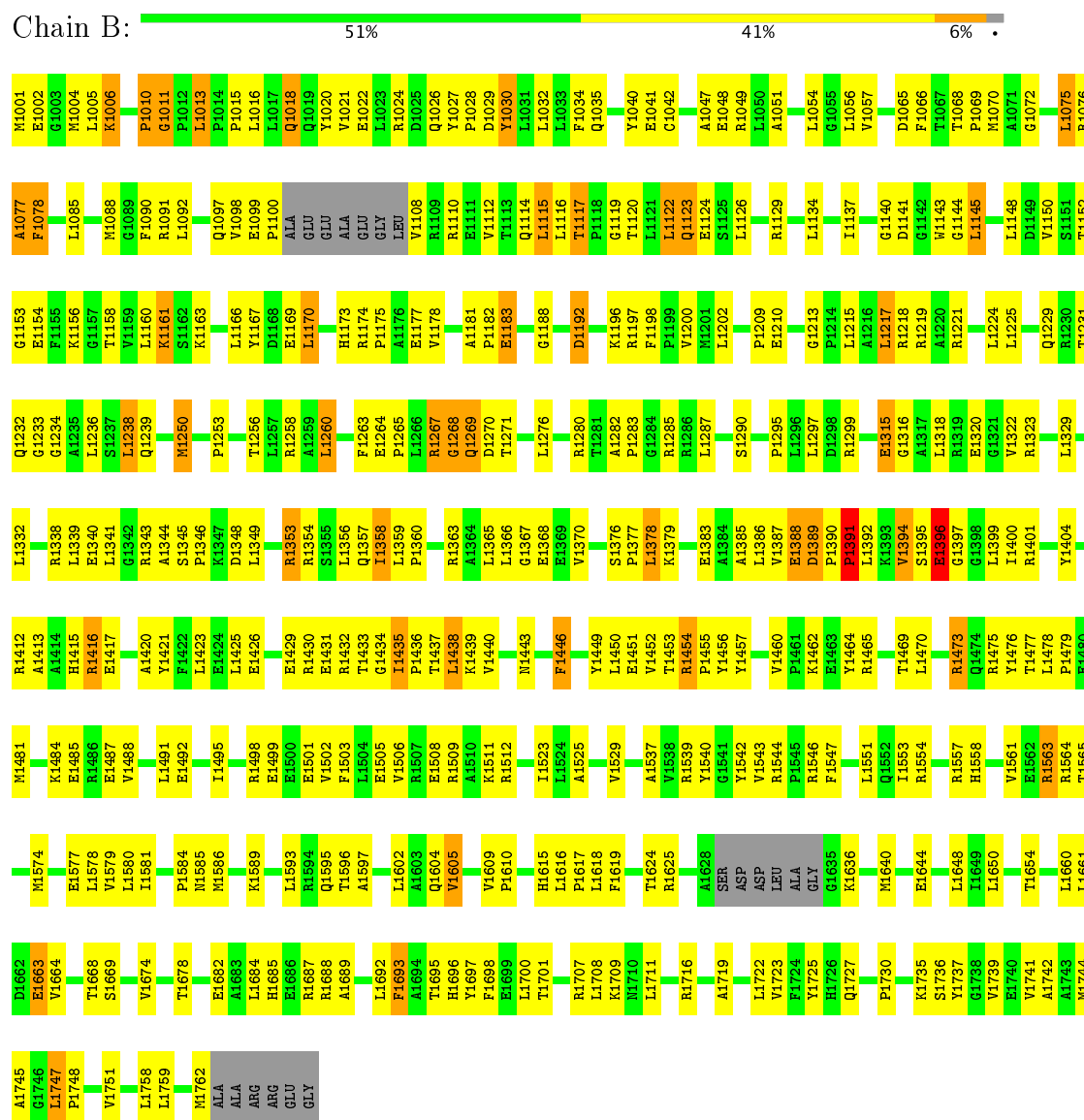
- Molecule 3: DNA MISMATCH REPAIR PROTEIN MUTS

Chain A: 





• Molecule 3: DNA MISMATCH REPAIR PROTEIN MUTS



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.72Å 113.50Å 160.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.17 – 2.70	Depositor
% Data completeness (in resolution range)	90.8 (23.17-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13165	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, 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	C	0.32	0/525	0.66	0/809
2	D	0.29	0/505	0.66	0/778
3	A	0.39	0/6111	0.66	1/8249 (0.0%)
3	B	0.39	0/6040	0.68	2/8152 (0.0%)
All	All	0.38	0/13181	0.67	3/17988 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1268	GLY	N-CA-C	-5.30	99.86	113.10
3	A	134	LEU	N-CA-C	-5.13	97.14	111.00
3	B	1329	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	469	0	259	35	0
2	D	450	0	246	38	0
3	A	6006	0	6093	362	0
3	B	5936	0	6023	381	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	27	0	12	2	0
6	B	27	0	12	3	0
7	A	105	0	0	13	0
7	B	115	0	0	20	0
7	C	4	0	0	6	0
7	D	4	0	0	0	0
All	All	13165	0	12645	798	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 31.

All (798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1663:GLU:HG3	7:B:150:HOH:O	1.40	1.18
3:B:1597:ALA:HB2	3:B:1660:LEU:HD11	1.34	1.10
3:A:267:ARG:HB2	3:A:269:GLN:HE21	1.12	1.07
1:C:1916:DG:H2''	1:C:1917:DG:H5'	1.35	1.07
3:B:1723:VAL:HG13	7:B:149:HOH:O	1.54	1.06
3:B:1117:THR:HG23	3:B:1177:GLU:OE1	1.60	1.00
3:B:1001:MSE:HE3	3:B:1004:MSE:HG3	1.44	0.98
3:A:59:THR:HG22	3:A:60:HIS:H	1.27	0.96
3:A:722:LEU:H	3:A:744:MSE:HE1	1.31	0.95
3:A:174:ARG:HE	3:A:174:ARG:HA	1.31	0.94
3:B:1368:GLU:HG2	7:B:163:HOH:O	1.67	0.94
2:D:1967:DG:H2''	2:D:1968:DC:H5''	1.50	0.92
3:B:1574:MSE:HE3	3:B:1579:VAL:HG23	1.51	0.92
3:A:267:ARG:O	3:A:269:GLN:HG3	1.71	0.88
3:A:267:ARG:HB2	3:A:269:GLN:NE2	1.86	0.88
1:C:1909:DA:H5''	3:B:1453:THR:HB	1.55	0.87
3:B:1269:GLN:NE2	3:B:1270:ASP:H	1.73	0.87
3:A:581:ILE:HD11	3:A:692:LEU:HD22	1.55	0.86
3:A:35:GLN:HG3	3:A:97:GLN:HG3	1.58	0.86
3:A:201:MSE:HE3	3:A:203:SER:OG	1.78	0.84
3:B:1553:ILE:HD11	3:B:1616:LEU:HD21	1.60	0.83
1:C:1916:DG:N7	7:C:195:HOH:O	2.11	0.83
3:A:172:ARG:O	3:A:293:ARG:HD3	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:722:LEU:H	3:A:744:MSE:CE	1.93	0.81
3:A:519:GLU:HG3	3:A:522:ARG:HH11	1.45	0.81
3:A:161:LYS:HD2	3:A:162:SER:H	1.46	0.81
3:A:722:LEU:HB2	3:A:744:MSE:HE1	1.61	0.81
3:A:161:LYS:HD2	3:A:162:SER:N	1.96	0.81
3:B:1593:LEU:HD22	3:B:1692:LEU:HB3	1.62	0.81
1:C:1909:DA:H2''	1:C:1910:DG:H5'	1.63	0.80
3:A:595:GLN:NE2	7:A:1954:HOH:O	2.12	0.80
2:D:1958:DC:H4'	3:B:1443:ASN:HD21	1.46	0.80
1:C:1903:DG:H2''	1:C:1904:DA:C5'	2.12	0.79
3:B:1397:GLY:HA2	3:B:1499:GLU:OE1	1.82	0.79
3:B:1027:TYR:CE1	3:B:1112:VAL:HG21	2.17	0.79
3:B:1076:ARG:HG3	3:B:1077:ALA:H	1.47	0.79
3:A:497:ARG:O	3:A:501:GLU:HG3	1.83	0.79
3:B:1018:GLN:O	3:B:1022:GLU:HG3	1.83	0.78
6:B:1999:ADP:H3'	7:B:165:HOH:O	1.81	0.78
3:A:322:VAL:HG11	3:A:527:LEU:HD22	1.63	0.78
3:B:1085:LEU:O	3:B:1090:PHE:HB2	1.83	0.78
3:A:672:ASP:O	3:A:676:ILE:HG12	1.84	0.78
3:A:171:PHE:CD2	3:A:254:GLU:HG3	2.19	0.78
3:A:674:VAL:CG1	3:A:699:GLU:HG3	2.15	0.77
2:D:1956:DA:OP1	3:B:1108:VAL:HG22	1.85	0.77
3:B:1685:HIS:HE1	3:B:1707:ARG:H	1.32	0.77
3:A:394:VAL:HG21	3:A:500:GLU:HA	1.67	0.77
3:B:1057:VAL:HG23	7:B:219:HOH:O	1.83	0.77
3:A:51:ALA:HA	3:A:56:LEU:HB2	1.67	0.76
3:B:1034:PHE:CZ	3:B:1110:ARG:HD2	2.21	0.76
3:B:1439:LYS:HB2	3:B:1451:GLU:HB3	1.67	0.76
2:D:1962:DC:H1'	2:D:1963:DG:H5''	1.68	0.76
3:A:722:LEU:N	3:A:744:MSE:HE1	2.00	0.75
3:B:1318:LEU:HD12	3:B:1365:LEU:HD22	1.68	0.75
3:B:1097:GLN:NE2	3:B:1110:ARG:HH21	1.85	0.74
1:C:1903:DG:H2''	1:C:1904:DA:H5'	1.69	0.74
3:A:353:ARG:O	3:A:357:GLN:HG3	1.88	0.73
3:B:1379:LYS:O	3:B:1383:GLU:HG3	1.88	0.73
3:A:35:GLN:HB3	3:A:95:ALA:O	1.89	0.73
3:B:1160:LEU:HD22	3:B:1166:LEU:HA	1.69	0.73
3:A:256:THR:O	3:A:260:LEU:HB2	1.88	0.73
3:B:1005:LEU:HD21	3:B:1068:THR:HG21	1.69	0.72
3:B:1129:ARG:HD2	3:B:1285:ARG:NH1	2.04	0.72
1:C:1916:DG:H4'	7:C:211:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:328:ARG:O	3:A:354:ARG:NH1	2.23	0.72
3:A:493:ALA:HA	3:A:496:ARG:NH1	2.05	0.72
3:A:368:GLU:CB	7:A:1927:HOH:O	2.37	0.72
3:B:1574:MSE:HE3	3:B:1579:VAL:CG2	2.19	0.72
3:B:1316:GLY:O	3:B:1320:GLU:HG3	1.90	0.71
3:B:1122:LEU:H	3:B:1123:GLN:NE2	1.89	0.71
3:B:1454:ARG:HH11	3:B:1454:ARG:HG2	1.55	0.71
3:B:1433:THR:HG22	3:B:1435:ILE:HG13	1.71	0.71
3:B:1280:ARG:HG3	3:B:1280:ARG:HH11	1.55	0.71
3:A:507:ARG:HD2	7:A:1876:HOH:O	1.91	0.70
3:A:585:ASN:O	3:A:586:MSE:HB2	1.91	0.70
3:A:593:LEU:CD2	3:A:692:LEU:HB3	2.21	0.70
2:D:1967:DG:C2'	2:D:1968:DC:H5''	2.19	0.70
3:A:759:LEU:HA	3:A:762:MSE:HE2	1.73	0.70
3:B:1229:GLN:HG2	3:B:1236:LEU:HG	1.74	0.70
3:B:1395:SER:O	3:B:1396:GLU:HB2	1.91	0.70
3:A:758:LEU:O	3:A:762:MSE:HG3	1.92	0.70
1:C:1916:DG:H2''	7:C:146:HOH:O	1.92	0.70
3:A:405:ASP:HB3	3:A:408:LEU:HB3	1.73	0.70
3:A:328:ARG:HB2	3:A:358:ILE:HD11	1.74	0.69
3:B:1426:GLU:O	3:B:1430:ARG:HG2	1.92	0.69
2:D:1968:DC:H2''	2:D:1969:DG:O5'	1.92	0.69
3:B:1456:TYR:O	3:B:1460:VAL:HG23	1.92	0.69
3:B:1446:PHE:HB2	7:B:58:HOH:O	1.92	0.69
3:A:438:LEU:HD21	3:A:450:LEU:HD22	1.73	0.69
3:A:563:ARG:HA	3:A:563:ARG:NE	2.08	0.69
1:C:1916:DG:H2''	1:C:1917:DG:C5'	2.18	0.69
3:B:1122:LEU:H	3:B:1123:GLN:HE21	1.41	0.69
3:A:102:GLU:HG3	7:A:1895:HOH:O	1.92	0.68
3:B:1117:THR:CG2	3:B:1177:GLU:OE1	2.41	0.68
3:B:1124:GLU:HG2	7:B:185:HOH:O	1.92	0.68
3:A:593:LEU:HD22	3:A:692:LEU:HB3	1.73	0.68
3:A:60:HIS:CD2	3:A:60:HIS:N	2.62	0.68
3:B:1435:ILE:HG22	3:B:1438:LEU:H	1.59	0.68
3:A:59:THR:HG22	3:A:60:HIS:N	2.07	0.68
3:B:1097:GLN:HE21	3:B:1110:ARG:HH21	1.40	0.68
3:A:267:ARG:CB	3:A:269:GLN:HE21	2.01	0.67
3:B:1338:ARG:NH1	7:B:185:HOH:O	2.26	0.67
3:A:115:LEU:HB2	3:A:231:THR:HA	1.77	0.67
3:A:92:LEU:HD12	3:A:116:LEU:HD12	1.76	0.67
3:A:547:PHE:HA	3:A:616:LEU:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1010:PRO:HG2	3:B:1011:GLY:H	1.60	0.67
3:B:1123:GLN:HG3	3:B:1126:LEU:HD12	1.76	0.67
3:B:1460:VAL:HG11	3:B:1476:TYR:CZ	2.30	0.67
3:A:140:GLY:O	3:A:141:ASP:HB2	1.95	0.66
3:A:336:ALA:O	3:A:340:GLU:HG3	1.95	0.66
3:B:1376:SER:OG	3:B:1377:PRO:HD3	1.96	0.66
3:A:411:LEU:HB3	3:A:495:ILE:HG12	1.77	0.66
3:A:550:ARG:HH11	3:A:550:ARG:HG3	1.60	0.66
3:A:636:LYS:HE3	3:A:636:LYS:HA	1.76	0.66
3:B:1585:ASN:O	3:B:1586:MSE:HB2	1.95	0.66
3:B:1604:GLN:HE22	3:B:1619:PHE:H	1.44	0.66
3:A:555:ALA:HB3	3:A:612:GLU:HB2	1.77	0.66
3:B:1269:GLN:CG	3:B:1270:ASP:H	2.09	0.66
3:A:363:ARG:HH22	3:A:374:ASP:CA	2.09	0.66
3:A:5:LEU:HD11	3:A:44:GLY:HA3	1.77	0.66
3:A:308:ARG:HH11	3:A:308:ARG:CG	2.09	0.65
1:C:1921:DG:OP1	3:A:471:LYS:HE3	1.95	0.65
3:B:1140:GLY:HA3	7:B:70:HOH:O	1.95	0.65
3:B:1027:TYR:HE1	3:B:1112:VAL:HG21	1.61	0.65
3:B:1269:GLN:CD	3:B:1270:ASP:H	1.98	0.65
1:C:1916:DG:C2'	7:C:146:HOH:O	2.43	0.65
3:A:506:VAL:O	3:A:509:ARG:HB2	1.97	0.65
3:B:1353:ARG:O	3:B:1357:GLN:HG3	1.97	0.65
3:A:155:PHE:CZ	3:A:221:ARG:HG3	2.32	0.65
3:B:1737:TYR:O	3:B:1741:VAL:HG23	1.97	0.65
2:D:1955:DG:OP1	3:B:1015:PRO:HG2	1.96	0.65
3:A:678:THR:O	3:A:682:GLU:HG3	1.96	0.65
3:A:677:ALA:HB1	3:A:700:LEU:HD11	1.77	0.65
3:B:1747:LEU:CD1	3:B:1748:PRO:HD2	2.26	0.65
2:D:1962:DC:H2''	2:D:1963:DG:C5'	2.27	0.65
3:A:519:GLU:HG3	3:A:522:ARG:NH1	2.12	0.65
1:C:1905:DC:H2''	1:C:1906:DG:H5'	1.77	0.65
3:B:1435:ILE:HG12	3:B:1456:TYR:HD2	1.61	0.64
3:B:1269:GLN:O	3:B:1270:ASP:HB2	1.98	0.64
3:B:1387:VAL:HG23	3:B:1399:LEU:O	1.98	0.64
1:C:1901:DG:H1'	1:C:1902:DC:H5''	1.80	0.64
3:A:440:VAL:HG22	3:A:450:LEU:HD23	1.78	0.64
3:A:588:GLY:HA2	6:A:999:ADP:O2A	1.96	0.64
3:A:177:GLU:HG3	3:A:201:MSE:HE2	1.80	0.64
3:B:1011:GLY:HA3	3:B:1065:ASP:HB3	1.80	0.64
3:B:1674:VAL:HG22	3:B:1697:TYR:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1152:THR:HG22	3:B:1154:GLU:H	1.62	0.64
3:B:1363:ARG:NH2	3:B:1368:GLU:HB2	2.12	0.64
3:B:1435:ILE:HG12	3:B:1456:TYR:CD2	2.32	0.64
3:B:1525:ALA:O	3:B:1529:VAL:HG23	1.97	0.64
3:A:636:LYS:HB2	3:B:1586:MSE:HE3	1.80	0.64
3:A:396:GLU:HG3	3:A:397:GLY:N	2.13	0.63
3:B:1450:LEU:HD13	3:B:1464:TYR:CE2	2.33	0.63
1:C:1903:DG:H2''	1:C:1904:DA:H5''	1.80	0.63
2:D:1965:DT:H2''	2:D:1966:DA:C8	2.34	0.63
3:B:1123:GLN:NE2	3:B:1123:GLN:H	1.96	0.63
3:B:1267:ARG:NE	3:B:1267:ARG:HA	2.12	0.63
3:A:331:ASP:OD2	3:A:334:ARG:HD2	1.99	0.63
3:A:12:PRO:HD2	3:A:65:ASP:OD1	1.98	0.63
3:A:363:ARG:HH22	3:A:374:ASP:HA	1.62	0.63
3:B:1340:GLU:HA	3:B:1511:LYS:HE2	1.81	0.63
3:B:1477:THR:CG2	3:B:1478:LEU:N	2.61	0.63
3:B:1585:ASN:ND2	3:B:1589:LYS:NZ	2.45	0.63
3:A:448:TYR:HD1	3:A:485:GLU:HG3	1.63	0.63
3:A:636:LYS:HB3	3:B:1586:MSE:HG2	1.79	0.63
3:B:1114:GLN:O	3:B:1115:LEU:HD23	1.99	0.62
3:B:1356:LEU:O	3:B:1360:PRO:HD3	1.99	0.62
3:A:426:GLU:OE2	3:A:439:LYS:HA	1.99	0.62
3:A:498:ARG:O	3:A:502:VAL:HG23	2.00	0.62
3:A:765:ARG:HH11	3:A:765:ARG:HG2	1.64	0.62
2:D:1955:DG:OP1	2:D:1955:DG:H4'	1.99	0.62
3:B:1708:LEU:HD12	3:B:1709:LYS:H	1.63	0.62
3:B:1143:TRP:HZ3	3:B:1161:LYS:O	1.82	0.62
2:D:1962:DC:H2''	2:D:1963:DG:H5'	1.82	0.62
3:A:708:LEU:C	3:A:708:LEU:HD23	2.20	0.62
3:B:1318:LEU:O	3:B:1322:VAL:HG23	2.00	0.62
3:A:100:PRO:HG2	3:A:103:GLU:CG	2.30	0.62
3:B:1747:LEU:HD13	3:B:1748:PRO:HD2	1.81	0.62
3:B:1454:ARG:HH11	3:B:1457:TYR:HE2	1.48	0.61
3:B:1066:PHE:HE2	3:B:1068:THR:HB	1.64	0.61
3:B:1388:GLU:HG3	3:B:1401:ARG:HH22	1.65	0.61
3:B:1354:ARG:CZ	3:B:1358:ILE:HD12	2.30	0.61
3:B:1236:LEU:HB2	3:B:1238:LEU:HD11	1.81	0.61
3:A:174:ARG:NE	3:A:174:ARG:HA	2.12	0.61
3:B:1363:ARG:HH11	3:B:1363:ARG:HG2	1.66	0.61
3:A:717:GLU:HG2	3:A:722:LEU:HD21	1.82	0.61
3:B:1711:LEU:HD23	3:B:1730:PRO:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:14:PRO:O	3:A:18:GLN:HB2	2.00	0.60
3:A:239:GLN:NE2	3:A:240:PRO:HD2	2.15	0.60
3:A:27:TYR:CE1	3:A:112:VAL:HG21	2.36	0.60
3:B:1029:ASP:HB3	3:B:1091:ARG:NH2	2.16	0.60
3:B:1158:THR:HG23	3:B:1160:LEU:HD11	1.83	0.60
3:B:1066:PHE:CE2	3:B:1068:THR:HB	2.37	0.60
3:B:1210:GLU:HG3	3:B:1225:LEU:HD12	1.81	0.60
3:B:1430:ARG:HB3	3:B:1435:ILE:O	2.02	0.60
3:B:1426:GLU:HG3	3:B:1440:VAL:HG23	1.82	0.60
3:A:114:GLN:HE22	3:A:123:GLN:HE22	1.48	0.60
3:A:454:ARG:HB3	3:A:455:PRO:HD3	1.83	0.60
3:B:1169:GLU:O	3:B:1173:HIS:HD2	1.83	0.60
3:A:376:SER:N	3:A:377:PRO:HD2	2.15	0.60
3:A:368:GLU:HB3	7:A:1927:HOH:O	1.97	0.60
3:B:1399:LEU:HD21	3:B:1503:PHE:CD1	2.36	0.60
3:B:1668:THR:OG1	3:B:1669:SER:N	2.35	0.60
3:A:318:LEU:HD11	3:A:366:LEU:HD23	1.84	0.60
3:A:574:MSE:HE3	3:A:579:VAL:HG23	1.82	0.60
3:B:1564:ARG:HD3	7:B:15:HOH:O	2.00	0.60
3:B:1678:THR:O	3:B:1682:GLU:HG3	2.02	0.60
3:A:479:PRO:HA	3:A:482:LYS:NZ	2.16	0.60
3:B:1183:GLU:OE2	3:B:1219:ARG:NH2	2.29	0.60
3:A:380:GLU:OE2	7:A:1948:HOH:O	2.15	0.60
3:A:487:GLU:OE1	7:A:1946:HOH:O	2.17	0.60
3:B:1013:LEU:HD21	3:B:1021:VAL:HG21	1.84	0.60
3:B:1698:PHE:O	3:B:1701:THR:HB	2.01	0.60
3:B:1589:LYS:HE3	6:B:1999:ADP:O1B	2.01	0.60
3:B:1076:ARG:HG3	3:B:1077:ALA:N	2.17	0.59
3:B:1366:LEU:HD13	3:B:1370:VAL:HG21	1.82	0.59
3:B:1636:LYS:HG2	3:B:1640:MSE:HE3	1.84	0.59
3:A:415:HIS:O	3:A:419:VAL:HG23	2.01	0.59
3:A:509:ARG:HE	3:A:509:ARG:HA	1.68	0.59
3:B:1269:GLN:HE21	3:B:1270:ASP:H	1.49	0.59
3:B:1389:ASP:OD1	3:B:1389:ASP:O	2.20	0.59
3:B:1454:ARG:HA	3:B:1457:TYR:CE2	2.38	0.59
3:B:1624:THR:HG22	3:B:1660:LEU:HD12	1.83	0.59
3:A:748:PRO:HB2	3:A:751:VAL:HG23	1.85	0.59
3:B:1097:GLN:HG2	3:B:1110:ARG:NE	2.18	0.59
3:B:1258:ARG:HH11	3:B:1258:ARG:HG2	1.68	0.59
3:A:394:VAL:HG13	3:A:395:SER:N	2.17	0.59
3:A:308:ARG:HH11	3:A:308:ARG:HG2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:493:ALA:HA	3:A:496:ARG:HH12	1.67	0.58
3:A:554:ARG:O	3:A:555:ALA:HB3	2.03	0.58
2:D:1967:DG:H2''	2:D:1968:DC:C5'	2.30	0.58
3:B:1160:LEU:HD12	3:B:1160:LEU:N	2.18	0.58
1:C:1921:DG:H2'	1:C:1922:DT:H71	1.86	0.58
3:A:548:GLY:O	3:A:617:PRO:HA	2.03	0.58
3:B:1178:VAL:HG23	3:B:1200:VAL:HG11	1.85	0.58
3:B:1685:HIS:O	3:B:1707:ARG:NH2	2.33	0.58
3:B:1282:ALA:HB3	3:B:1283:PRO:HD3	1.86	0.58
3:B:1636:LYS:CG	3:B:1640:MSE:HE3	2.33	0.58
3:A:160:LEU:N	3:A:160:LEU:HD12	2.19	0.58
2:D:1969:DG:H2''	2:D:1970:DT:C5'	2.33	0.58
3:A:130:GLU:OE2	3:A:285:ARG:HD3	2.03	0.58
3:A:76:ARG:NH1	3:A:76:ARG:HB3	2.19	0.58
3:B:1425:LEU:HD21	3:B:1481:MSE:SE	2.54	0.57
3:A:40:TYR:CE1	3:A:75:LEU:HD22	2.39	0.57
3:B:1001:MSE:HB3	3:B:1004:MSE:HB2	1.85	0.57
3:B:1716:ARG:HG3	3:B:1725:TYR:CE1	2.38	0.57
3:A:123:GLN:HB2	3:A:126:LEU:HD12	1.84	0.57
3:B:1547:PHE:HA	3:B:1616:LEU:O	2.05	0.57
3:B:1685:HIS:CE1	3:B:1707:ARG:H	2.17	0.57
3:A:155:PHE:HZ	3:A:221:ARG:HG3	1.69	0.57
3:A:583:GLY:O	3:A:589:LYS:NZ	2.35	0.57
2:D:1955:DG:H2'	2:D:1956:DA:H8	1.68	0.57
3:A:356:LEU:HA	3:A:359:LEU:HD13	1.87	0.57
2:D:1960:DG:H2''	2:D:1961:DC:OP2	2.04	0.57
3:B:1065:ASP:OD1	7:B:156:HOH:O	2.18	0.57
3:A:405:ASP:OD1	3:A:498:ARG:NE	2.34	0.57
3:B:1434:GLY:O	3:B:1436:PRO:HD3	2.05	0.57
3:B:1346:PRO:HB3	3:B:1399:LEU:HD11	1.85	0.57
1:C:1917:DG:H5'	7:C:146:HOH:O	2.04	0.56
3:A:174:ARG:CA	3:A:174:ARG:HE	2.13	0.56
3:A:299:ARG:NH1	3:A:303:GLU:OE2	2.38	0.56
3:A:335:LEU:HD21	3:A:348:ASP:HB3	1.87	0.56
3:A:287:LEU:HD23	3:A:529:VAL:HG21	1.87	0.56
3:A:705:LEU:N	7:A:1854:HOH:O	2.37	0.56
3:B:1299:ARG:NH2	3:B:1547:PHE:O	2.38	0.56
3:A:674:VAL:HG13	3:A:699:GLU:HG3	1.87	0.56
3:B:1005:LEU:CD2	3:B:1068:THR:HG21	2.34	0.56
3:A:716:ARG:O	3:A:718:GLU:HG3	2.05	0.56
3:B:1388:GLU:HG3	3:B:1401:ARG:NH2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:GLN:HB3	3:A:96:ASP:HA	1.87	0.56
3:B:1200:VAL:O	3:B:1202:LEU:HD13	2.06	0.56
3:A:463:GLU:H	3:A:463:GLU:CD	2.08	0.56
3:B:1153:GLY:O	3:B:1239:GLN:HG2	2.06	0.56
3:B:1010:PRO:O	3:B:1011:GLY:O	2.24	0.56
2:D:1958:DC:C4'	3:B:1443:ASN:HD21	2.15	0.56
3:B:1758:LEU:O	3:B:1762:MSE:HG3	2.05	0.56
3:A:177:GLU:CD	3:A:201:MSE:HE2	2.26	0.56
1:C:1910:DG:OP1	3:B:1439:LYS:NZ	2.35	0.56
3:A:704:GLY:O	3:A:705:LEU:HD23	2.05	0.56
3:B:1585:ASN:HD22	3:B:1589:LYS:NZ	2.03	0.56
3:A:325:LEU:HD22	3:A:358:ILE:HG23	1.88	0.56
3:A:52:ARG:HG3	3:A:53:ALA:N	2.21	0.56
3:A:74:PRO:HB2	3:A:76:ARG:HG2	1.88	0.56
3:B:1554:ARG:HH11	3:B:1554:ARG:HG2	1.70	0.56
3:A:177:GLU:CG	3:A:201:MSE:HE2	2.36	0.55
3:B:1161:LYS:HD2	3:B:1161:LYS:N	2.21	0.55
3:B:1265:PRO:C	3:B:1267:ARG:H	2.09	0.55
3:B:1122:LEU:HD21	3:B:1341:LEU:HD13	1.87	0.55
3:A:392:LEU:HG	3:A:393:LYS:HG3	1.88	0.55
3:B:1120:THR:O	3:B:1150:VAL:HG21	2.07	0.55
3:A:114:GLN:NE2	3:A:123:GLN:HE22	2.04	0.55
3:A:24:ARG:HA	3:A:32:LEU:HD22	1.87	0.55
3:A:430:ARG:HD3	3:A:436:PRO:O	2.07	0.55
2:D:1962:DC:H5'	3:A:38:ASP:OD2	2.06	0.55
3:A:416:ARG:HH11	3:A:416:ARG:HG2	1.72	0.55
3:A:550:ARG:NH1	3:A:550:ARG:HG3	2.20	0.55
3:A:35:GLN:HG2	3:A:97:GLN:H	1.72	0.55
3:B:1215:LEU:O	3:B:1219:ARG:HG3	2.07	0.55
3:B:1625:ARG:O	3:B:1625:ARG:HG3	2.05	0.55
3:B:1145:LEU:HD21	3:B:1170:LEU:HD23	1.89	0.55
3:A:201:MSE:HE3	3:A:203:SER:HG	1.71	0.55
3:B:1250:MSE:HE3	3:B:1604:GLN:HB2	1.88	0.55
3:A:312:PHE:HB3	3:A:319:ARG:HG3	1.88	0.54
3:A:375:LEU:C	3:A:377:PRO:HD2	2.27	0.54
1:C:1916:DG:C4'	7:C:211:HOH:O	2.50	0.54
3:A:674:VAL:HG11	3:A:699:GLU:HG3	1.89	0.54
3:A:756:ARG:HH11	3:A:756:ARG:HG2	1.73	0.54
2:D:1955:DG:H2'	2:D:1956:DA:C8	2.42	0.54
3:B:1143:TRP:HB3	3:B:1166:LEU:HD13	1.90	0.54
3:B:1232:GLN:HG2	3:B:1341:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1597:ALA:HB2	3:B:1660:LEU:CD1	2.24	0.54
3:B:1110:ARG:HH11	3:B:1110:ARG:HG3	1.72	0.54
3:A:585:ASN:HD21	3:A:696:HIS:HE1	1.56	0.54
3:B:1054:LEU:HD23	3:B:1088:MSE:HE1	1.90	0.54
3:B:1385:ALA:HB2	3:B:1404:TYR:CE1	2.43	0.54
3:B:1450:LEU:O	3:B:1475:ARG:HA	2.07	0.54
3:B:1696:HIS:N	7:B:150:HOH:O	2.40	0.54
3:A:408:LEU:HD21	3:A:412:ARG:HH12	1.73	0.54
3:A:482:LYS:HD2	3:A:486:ARG:HH22	1.72	0.54
3:A:357:GLN:HG2	3:A:379:LYS:HD2	1.90	0.54
3:B:1114:GLN:HE21	3:B:1343:ARG:NH1	2.05	0.54
3:A:438:LEU:HD23	3:A:438:LEU:C	2.27	0.54
3:B:1097:GLN:HE21	3:B:1110:ARG:HE	1.56	0.54
3:B:1563:ARG:HA	3:B:1563:ARG:NH1	2.22	0.54
3:A:100:PRO:HG2	3:A:103:GLU:HG3	1.89	0.53
3:A:62:THR:HG23	3:A:67:THR:HB	1.91	0.53
3:B:1123:GLN:CG	3:B:1126:LEU:HD12	2.38	0.53
3:B:1357:GLN:O	3:B:1360:PRO:HD2	2.09	0.53
3:B:1449:TYR:HA	3:B:1481:MSE:HE1	1.91	0.53
3:A:92:LEU:HB2	3:A:116:LEU:HB2	1.89	0.53
3:B:1617:PRO:HG2	3:B:1619:PHE:CZ	2.43	0.53
2:D:1962:DC:C1'	2:D:1963:DG:H5''	2.37	0.53
3:A:299:ARG:O	3:A:303:GLU:HG2	2.09	0.53
3:B:1192:ASP:O	3:B:1196:LYS:HG3	2.09	0.53
3:B:1269:GLN:CG	3:B:1270:ASP:N	2.70	0.53
2:D:1969:DG:H2''	2:D:1970:DT:H5''	1.90	0.53
3:A:308:ARG:HH11	3:A:308:ARG:CB	2.22	0.53
3:B:1097:GLN:HE21	3:B:1110:ARG:NH2	2.05	0.53
3:B:1439:LYS:HD2	3:B:1451:GLU:OE1	2.08	0.53
3:A:379:LYS:HB3	3:A:379:LYS:NZ	2.24	0.53
3:A:663:GLU:O	3:A:666:ARG:HG2	2.09	0.53
3:B:1413:ALA:HA	3:B:1416:ARG:NH1	2.23	0.53
3:B:1454:ARG:NH1	3:B:1457:TYR:HE2	2.06	0.53
3:B:1477:THR:HG22	3:B:1478:LEU:N	2.24	0.53
1:C:1909:DA:H5''	3:B:1453:THR:CB	2.35	0.53
3:A:148:LEU:HD12	3:A:154:GLU:O	2.09	0.53
3:A:327:TYR:O	7:A:1936:HOH:O	2.19	0.53
3:A:551:LEU:HA	3:A:615:HIS:O	2.08	0.53
3:B:1129:ARG:HB3	3:B:1285:ARG:HD2	1.91	0.53
3:B:1353:ARG:HG3	3:B:1354:ARG:N	2.24	0.53
3:B:1356:LEU:HB3	3:B:1379:LYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1901:DG:H2''	1:C:1902:DC:H5''	1.90	0.53
3:A:114:GLN:HE22	3:A:123:GLN:NE2	2.06	0.53
3:B:1051:ALA:HA	3:B:1056:LEU:HB2	1.91	0.52
3:B:1024:ARG:HD2	3:B:1024:ARG:C	2.29	0.52
3:B:1040:TYR:CE1	3:B:1075:LEU:HD22	2.45	0.52
3:A:442:TYR:HE1	3:A:489:TYR:HH	1.57	0.52
3:A:557:ARG:HG3	3:A:610:PRO:HB2	1.90	0.52
3:A:642:GLU:OE2	3:A:666:ARG:NH1	2.40	0.52
3:B:1454:ARG:NH1	3:B:1454:ARG:HG2	2.23	0.52
3:B:1485:GLU:C	3:B:1487:GLU:H	2.12	0.52
3:B:1213:GLY:O	3:B:1218:ARG:HD2	2.10	0.52
3:B:1287:LEU:HD23	3:B:1529:VAL:HG21	1.91	0.52
3:B:1498:ARG:HD2	3:B:1501:GLU:OE1	2.09	0.52
3:A:16:LEU:HD11	3:A:110:ARG:NH1	2.25	0.52
3:A:237:SER:OG	3:A:340:GLU:OE1	2.27	0.52
3:A:273:PHE:HD1	3:A:292:LEU:HD12	1.74	0.52
3:A:609:VAL:HB	3:A:610:PRO:HD2	1.91	0.52
3:B:1269:GLN:NE2	3:B:1270:ASP:N	2.52	0.52
3:B:1232:GLN:O	3:B:1234:GLY:N	2.42	0.52
3:B:1558:HIS:CD2	3:B:1561:VAL:H	2.28	0.52
3:A:756:ARG:O	3:A:760:GLN:HG3	2.10	0.52
3:B:1363:ARG:HG2	3:B:1363:ARG:NH1	2.22	0.52
2:D:1970:DT:H2''	2:D:1971:DC:C5	2.45	0.52
3:A:734:SER:HB2	3:A:735:LYS:HD3	1.92	0.52
3:A:354:ARG:HH11	3:A:354:ARG:HG2	1.73	0.52
3:A:574:MSE:HG2	3:A:579:VAL:HG21	1.92	0.52
3:B:1551:LEU:HD23	3:B:1551:LEU:C	2.31	0.52
3:A:661:LEU:HD13	3:A:664:VAL:HG21	1.92	0.51
3:B:1299:ARG:HH21	3:B:1547:PHE:HB2	1.73	0.51
3:A:386:LEU:O	3:A:401:ARG:HG3	2.11	0.51
3:B:1426:GLU:HG2	3:B:1430:ARG:CZ	2.40	0.51
3:A:431:GLU:OE1	3:A:431:GLU:HA	2.10	0.51
3:A:535:GLU:HG3	3:A:539:ARG:HH12	1.74	0.51
3:A:636:LYS:CB	3:B:1586:MSE:HE3	2.40	0.51
3:B:1363:ARG:HH22	3:B:1368:GLU:HB2	1.75	0.51
2:D:1961:DC:H2'	2:D:1962:DC:C5	2.46	0.51
3:A:6:LYS:HD3	3:A:45:GLU:HG2	1.92	0.51
3:A:557:ARG:NE	3:A:562:GLU:OE2	2.42	0.51
3:B:1453:THR:OG1	3:B:1455:PRO:HD2	2.10	0.51
3:A:172:ARG:HH22	3:A:252:LEU:H	1.57	0.51
3:A:394:VAL:HG21	3:A:500:GLU:CA	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:GLN:HG2	3:A:97:GLN:N	2.25	0.51
3:B:1011:GLY:HA3	3:B:1065:ASP:CB	2.40	0.51
3:B:1167:TYR:CD2	3:B:1198:PHE:HE1	2.29	0.51
3:B:1129:ARG:HD2	3:B:1285:ARG:CZ	2.41	0.51
3:B:1585:ASN:ND2	3:B:1589:LYS:HZ3	2.07	0.51
3:B:1502:VAL:O	3:B:1506:VAL:HG23	2.10	0.51
3:B:1580:LEU:HD12	3:B:1701:THR:HA	1.93	0.51
1:C:1901:DG:C2'	1:C:1902:DC:H5''	2.41	0.51
2:D:1962:DC:C2'	2:D:1963:DG:H5''	2.41	0.51
3:B:1435:ILE:C	3:B:1437:THR:H	2.14	0.51
1:C:1902:DC:H2''	1:C:1903:DG:C8	2.45	0.50
1:C:1904:DA:H2	2:D:1971:DC:O2	1.94	0.50
3:A:160:LEU:HD23	3:A:165:ALA:HB1	1.94	0.50
3:A:172:ARG:O	3:A:293:ARG:CD	2.57	0.50
3:A:271:THR:O	3:A:275:VAL:HG23	2.11	0.50
3:A:685:HIS:HE1	3:A:707:ARG:H	1.58	0.50
3:A:59:THR:CG2	3:A:60:HIS:H	2.10	0.50
3:A:676:ILE:O	3:A:680:VAL:HG23	2.11	0.50
3:B:1030:TYR:N	3:B:1030:TYR:CD1	2.78	0.50
3:B:1434:GLY:O	3:B:1436:PRO:CD	2.60	0.50
3:B:1585:ASN:ND2	3:B:1589:LYS:HZ1	2.08	0.50
3:B:1098:VAL:O	3:B:1099:GLU:C	2.49	0.50
3:B:1363:ARG:HH12	3:B:1367:GLY:HA2	1.75	0.50
1:C:1917:DG:H2''	1:C:1918:DC:OP2	2.11	0.50
3:B:1092:LEU:HB2	3:B:1116:LEU:HB2	1.94	0.50
3:A:169:GLU:O	3:A:173:HIS:HD2	1.94	0.50
3:A:461:PRO:HG2	3:A:464:TYR:CD1	2.46	0.50
3:A:170:LEU:HD12	3:A:198:PHE:CE2	2.47	0.50
3:A:83:GLU:CG	3:A:87:LYS:HE2	2.42	0.50
3:B:1450:LEU:HD13	3:B:1464:TYR:CZ	2.46	0.50
3:B:1578:LEU:HD23	3:B:1708:LEU:HD13	1.94	0.50
3:B:1415:HIS:CE1	3:B:1492:GLU:HG2	2.47	0.50
3:B:1685:HIS:HE1	3:B:1707:ARG:N	2.06	0.50
1:C:1912:DG:O6	2:D:1962:DC:N4	2.43	0.50
3:A:256:THR:CG2	3:A:260:LEU:HD22	2.42	0.49
3:A:580:LEU:HD23	3:A:693:PHE:HB3	1.94	0.49
3:A:670:SER:O	3:A:674:VAL:HG23	2.12	0.49
3:B:1110:ARG:NH1	3:B:1110:ARG:HG3	2.27	0.49
3:A:379:LYS:HZ3	3:A:379:LYS:HB3	1.77	0.49
3:A:581:ILE:HG22	3:A:589:LYS:HG2	1.95	0.49
3:B:1258:ARG:NH1	3:B:1258:ARG:HG2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1604:GLN:HE22	3:B:1619:PHE:N	2.10	0.49
3:B:1640:MSE:O	3:B:1644:GLU:HG3	2.13	0.49
3:B:1354:ARG:HD2	7:B:201:HOH:O	2.12	0.49
3:B:1357:GLN:HA	3:B:1379:LYS:HD2	1.95	0.49
1:C:1912:DG:H2''	1:C:1913:DT:OP2	2.12	0.49
3:A:308:ARG:HH11	3:A:308:ARG:HB3	1.76	0.49
3:A:156:LYS:NZ	3:A:173:HIS:HE1	2.11	0.49
3:A:467:VAL:HG21	3:A:477:THR:OG1	2.13	0.49
3:A:595:GLN:O	3:A:599:ILE:HG13	2.12	0.49
3:B:1115:LEU:HB2	3:B:1231:THR:HA	1.94	0.49
3:B:1359:LEU:HB3	3:B:1360:PRO:HD3	1.94	0.49
6:B:1999:ADP:C3'	7:B:165:HOH:O	2.52	0.49
3:A:554:ARG:NH1	3:A:613:GLU:OE2	2.46	0.49
3:B:1270:ASP:HB2	7:B:15:HOH:O	2.12	0.49
3:B:1353:ARG:NH2	3:B:1388:GLU:HA	2.28	0.49
3:A:722:LEU:CB	3:A:744:MSE:HE1	2.37	0.48
3:A:35:GLN:NE2	3:A:37:GLY:O	2.46	0.48
3:A:482:LYS:HG2	3:A:486:ARG:HH12	1.78	0.48
3:B:1478:LEU:HG	3:B:1479:PRO:HD2	1.95	0.48
3:B:1150:VAL:HG22	7:B:46:HOH:O	2.13	0.48
3:B:1469:THR:C	3:B:1470:LEU:HD12	2.33	0.48
3:B:1654:THR:O	3:B:1689:ALA:HB2	2.12	0.48
3:B:1579:VAL:HB	3:B:1692:LEU:HD23	1.95	0.48
3:A:24:ARG:HD2	3:A:46:ASP:OD2	2.13	0.48
3:A:535:GLU:CG	3:A:539:ARG:HH12	2.26	0.48
3:B:1551:LEU:HD21	3:B:1553:ILE:HD12	1.95	0.48
3:B:1636:LYS:HG2	3:B:1640:MSE:CE	2.43	0.48
3:A:668:THR:HG23	3:A:669:SER:N	2.29	0.48
3:A:718:GLU:O	3:A:719:ALA:C	2.51	0.48
3:B:1584:PRO:HB3	3:B:1737:TYR:CD1	2.49	0.48
3:A:366:LEU:CD1	3:A:527:LEU:HD11	2.44	0.48
3:A:540:TYR:O	3:A:557:ARG:NH2	2.47	0.48
3:A:557:ARG:HA	3:A:567:PHE:CE2	2.48	0.48
3:A:586:MSE:SE	3:B:1640:MSE:HE2	2.64	0.48
3:B:1097:GLN:NE2	3:B:1110:ARG:NH2	2.60	0.48
3:B:1297:LEU:O	3:B:1618:LEU:HD13	2.14	0.48
3:A:297:LEU:O	3:A:618:LEU:HD13	2.12	0.48
3:A:642:GLU:O	3:A:646:VAL:HG23	2.13	0.48
3:A:95:ALA:HA	3:A:112:VAL:HA	1.94	0.48
2:D:1959:DC:H2''	2:D:1960:DG:H5'	1.96	0.48
3:A:145:LEU:HD11	3:A:147:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:539:ARG:HG2	3:A:540:TYR:CE2	2.48	0.48
3:A:588:GLY:CA	6:A:999:ADP:O2A	2.62	0.48
3:B:1543:VAL:HG12	3:B:1544:ARG:N	2.29	0.48
3:A:421:TYR:CE1	3:A:484:LYS:HG3	2.48	0.48
3:B:1232:GLN:OE1	3:B:1343:ARG:NE	2.46	0.48
3:B:1615:HIS:CD2	3:B:1615:HIS:N	2.82	0.48
3:B:1429:GLU:O	3:B:1432:ARG:N	2.47	0.47
3:A:487:GLU:O	3:A:491:LEU:HG	2.14	0.47
3:A:276:LEU:O	3:A:536:VAL:HG21	2.14	0.47
3:A:554:ARG:NH2	3:A:612:GLU:OE1	2.47	0.47
3:B:1174:ARG:HD3	3:B:1174:ARG:HA	1.69	0.47
3:B:1470:LEU:N	3:B:1470:LEU:HD12	2.30	0.47
3:B:1604:GLN:NE2	3:B:1619:PHE:H	2.11	0.47
3:A:249:PHE:CG	3:A:294:HIS:HB3	2.50	0.47
3:A:525:ALA:O	3:A:529:VAL:HG23	2.14	0.47
3:B:1433:THR:HG22	3:B:1433:THR:O	2.14	0.47
3:B:1687:ARG:O	3:B:1688:ARG:HB2	2.14	0.47
1:C:1921:DG:C2'	1:C:1922:DT:H71	2.44	0.47
3:B:1688:ARG:NH2	3:B:1707:ARG:NH1	2.62	0.47
3:B:1026:GLN:O	3:B:1028:PRO:HD2	2.15	0.47
3:B:1181:ALA:HB1	3:B:1183:GLU:OE1	2.15	0.47
3:A:43:PHE:HA	3:A:47:ALA:HB2	1.97	0.47
3:A:479:PRO:HA	3:A:482:LYS:HZ3	1.78	0.47
3:B:1394:VAL:O	3:B:1395:SER:HB3	2.15	0.47
3:B:1539:ARG:HD2	3:B:1540:TYR:CZ	2.49	0.47
3:A:83:GLU:O	3:A:87:LYS:HG3	2.14	0.47
3:B:1022:GLU:O	3:B:1026:GLN:HG3	2.14	0.47
3:B:1412:ARG:O	3:B:1416:ARG:HG3	2.15	0.47
3:A:635:GLY:HA2	3:A:640:MSE:SE	2.65	0.47
3:A:734:SER:CB	3:A:735:LYS:HD3	2.44	0.47
3:B:1042:CYS:O	3:B:1047:ALA:HB2	2.15	0.47
3:B:1661:LEU:HD22	3:B:1664:VAL:HG21	1.97	0.47
3:A:135:ALA:HB3	3:A:178:VAL:HG22	1.96	0.47
3:A:442:TYR:HE1	3:A:489:TYR:OH	1.97	0.47
3:B:1452:VAL:O	3:B:1473:ARG:HB2	2.14	0.47
3:B:1663:GLU:CG	7:B:150:HOH:O	2.24	0.47
3:A:324:ARG:HD2	7:A:1856:HOH:O	2.14	0.46
3:B:1387:VAL:C	3:B:1389:ASP:H	2.19	0.46
3:A:129:ARG:HD3	3:A:285:ARG:NH1	2.30	0.46
3:A:225:LEU:HD21	3:A:238:LEU:HD11	1.96	0.46
3:A:225:LEU:CD2	3:A:238:LEU:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:308:ARG:HG2	3:A:308:ARG:NH1	2.26	0.46
3:A:376:SER:O	3:A:380:GLU:HG3	2.15	0.46
3:B:1346:PRO:HD2	3:B:1392:LEU:HA	1.97	0.46
3:B:1345:SER:O	3:B:1348:ASP:HB2	2.14	0.46
3:B:1470:LEU:CD2	3:B:1473:ARG:HE	2.28	0.46
3:B:1473:ARG:HD3	3:B:1473:ARG:N	2.30	0.46
3:B:1692:LEU:HD23	3:B:1692:LEU:HA	1.69	0.46
1:C:1918:DC:H2''	1:C:1919:DT:H5'	1.96	0.46
3:A:171:PHE:CE2	3:A:254:GLU:HG3	2.49	0.46
3:B:1269:GLN:HG3	3:B:1270:ASP:H	1.80	0.46
3:B:1417:GLU:O	3:B:1420:ALA:HB3	2.14	0.46
3:B:1722:LEU:HB2	3:B:1744:MSE:CE	2.46	0.46
3:A:187:ASN:OD1	3:A:189:ALA:HB3	2.15	0.46
3:A:335:LEU:HD21	3:A:348:ASP:CB	2.45	0.46
3:A:35:GLN:O	3:A:35:GLN:HG3	2.15	0.46
3:A:623:TYR:CE2	3:A:652:GLU:OE2	2.69	0.46
3:B:1602:LEU:O	3:B:1605:VAL:HG12	2.15	0.46
3:B:1685:HIS:CE1	3:B:1707:ARG:HB2	2.50	0.46
3:B:1747:LEU:HD12	3:B:1748:PRO:HD2	1.96	0.46
3:A:258:ARG:HH11	3:A:258:ARG:HG2	1.80	0.46
3:A:377:PRO:HG2	3:A:378:LEU:H	1.80	0.46
3:A:454:ARG:HA	3:A:457:TYR:CE1	2.50	0.46
3:B:1363:ARG:NH1	3:B:1367:GLY:HA2	2.30	0.46
3:A:24:ARG:CA	3:A:32:LEU:HD22	2.46	0.46
3:A:412:ARG:O	3:A:416:ARG:HG3	2.16	0.46
3:A:6:LYS:HE2	3:A:48:GLU:OE1	2.15	0.46
3:B:1485:GLU:C	3:B:1487:GLU:N	2.68	0.46
3:A:322:VAL:O	3:A:326:LEU:HG	2.15	0.46
3:A:58:LEU:HD23	3:A:58:LEU:HA	1.76	0.46
3:A:85:LEU:HA	3:A:88:MSE:HE3	1.96	0.46
3:B:1558:HIS:CD2	3:B:1561:VAL:HG23	2.50	0.46
2:D:1955:DG:C2'	2:D:1956:DA:H8	2.29	0.46
3:A:200:VAL:HG12	3:A:201:MSE:N	2.30	0.45
3:B:1581:ILE:HA	3:B:1711:LEU:O	2.16	0.45
3:A:140:GLY:O	3:A:141:ASP:CB	2.62	0.45
3:A:191:LEU:HG	3:A:195:ARG:NH1	2.31	0.45
3:A:66:PHE:C	3:A:66:PHE:CD2	2.89	0.45
3:B:1040:TYR:CD1	3:B:1075:LEU:HD22	2.51	0.45
3:B:1123:GLN:HE21	3:B:1123:GLN:H	1.63	0.45
3:B:1551:LEU:HG	3:B:1616:LEU:HD23	1.97	0.45
3:A:533:LEU:HD22	3:A:607:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:586:MSE:SE	3:B:1640:MSE:CE	3.15	0.45
3:A:624:THR:HG22	3:A:660:LEU:HB2	1.97	0.45
3:B:1256:THR:HA	3:B:1624:THR:OG1	2.15	0.45
3:A:16:LEU:CD1	3:A:110:ARG:NH1	2.80	0.45
3:A:239:GLN:HE21	3:A:240:PRO:HD2	1.81	0.45
3:B:1016:LEU:HD11	3:B:1034:PHE:HE2	1.80	0.45
3:B:1152:THR:HG22	3:B:1154:GLU:N	2.31	0.45
3:B:1470:LEU:HD22	3:B:1473:ARG:NE	2.32	0.45
3:A:385:ALA:O	3:A:400:ILE:HA	2.16	0.45
3:A:704:GLY:HA2	7:A:1854:HOH:O	2.16	0.45
3:A:83:GLU:HG2	3:A:87:LYS:HE2	1.98	0.45
3:B:1006:LYS:NZ	3:B:1048:GLU:OE1	2.49	0.45
3:B:1356:LEU:HD11	3:B:1378:LEU:HD13	1.98	0.45
3:B:1735:LYS:HB3	3:B:1735:LYS:HE2	1.77	0.45
3:B:1181:ALA:HB1	3:B:1182:PRO:HD2	1.99	0.45
3:A:36:VAL:HG22	3:A:110:ARG:NH1	2.31	0.45
3:A:34:PHE:O	3:A:41:GLU:N	2.39	0.45
3:A:282:ALA:HB3	3:A:283:PRO:HD3	1.98	0.45
3:A:717:GLU:HG2	3:A:722:LEU:CD2	2.45	0.45
3:B:1200:VAL:O	3:B:1202:LEU:CD1	2.65	0.45
3:B:1509:ARG:HH11	3:B:1509:ARG:HG2	1.82	0.45
1:C:1908:DT:H3	2:D:1966:DA:H61	1.65	0.45
3:A:465:ARG:O	3:A:476:TYR:HA	2.17	0.45
3:B:1345:SER:HB2	3:B:1392:LEU:HD22	1.98	0.45
3:B:1537:ALA:HA	3:B:1542:TYR:HB2	1.99	0.45
3:A:183:GLU:CD	3:A:183:GLU:H	2.18	0.45
3:A:211:GLY:O	3:A:218:ARG:HD2	2.17	0.45
3:A:232:GLN:HG3	3:A:236:LEU:HD23	1.99	0.45
1:C:1907:DC:H2''	1:C:1908:DT:O5'	2.16	0.45
3:A:256:THR:HG22	3:A:260:LEU:HD22	1.98	0.44
3:A:580:LEU:HD13	3:A:701:THR:HA	1.99	0.44
3:B:1156:LYS:NZ	3:B:1173:HIS:HE1	2.15	0.44
3:B:1232:GLN:HG3	3:B:1232:GLN:O	2.17	0.44
3:B:1339:LEU:HD23	3:B:1344:ALA:CB	2.47	0.44
3:B:1636:LYS:CD	3:B:1640:MSE:HE3	2.47	0.44
3:A:390:PRO:HA	3:A:391:PRO:HD3	1.81	0.44
3:A:278:GLU:HG3	3:A:536:VAL:CG2	2.47	0.44
3:A:582:THR:O	3:A:712:HIS:HA	2.17	0.44
3:B:1287:LEU:O	3:B:1290:SER:HB3	2.17	0.44
3:A:309:VAL:O	3:A:313:VAL:HG23	2.18	0.44
3:A:440:VAL:HG22	3:A:450:LEU:CD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1076:ARG:CG	3:B:1077:ALA:H	2.25	0.44
3:B:1429:GLU:C	3:B:1431:GLU:N	2.70	0.44
3:A:393:LYS:O	3:A:396:GLU:HG2	2.17	0.44
3:A:468:GLN:NE2	3:A:475:ARG:HH11	2.14	0.44
3:A:551:LEU:O	3:A:573:GLU:HA	2.18	0.44
3:A:76:ARG:CB	3:A:76:ARG:HH11	2.30	0.44
3:B:1119:GLY:O	3:B:1134:LEU:HB2	2.17	0.44
3:B:1268:GLY:O	3:B:1269:GLN:O	2.35	0.44
3:B:1280:ARG:HG3	3:B:1280:ARG:NH1	2.27	0.44
3:B:1595:GLN:HG3	3:B:1596:THR:N	2.32	0.44
3:B:1663:GLU:OE1	3:B:1696:HIS:ND1	2.50	0.44
3:A:16:LEU:HD11	3:A:34:PHE:HE2	1.83	0.44
2:D:1959:DC:H1'	2:D:1960:DG:H5'	2.00	0.44
3:A:742:ALA:O	3:A:745:ALA:HB3	2.17	0.44
3:B:1020:TYR:CE1	3:B:1032:LEU:HD12	2.52	0.44
3:B:1396:GLU:HA	3:B:1396:GLU:OE1	2.18	0.44
3:A:26:GLN:C	3:A:28:PRO:HD3	2.38	0.44
3:A:482:LYS:CG	3:A:486:ARG:HH22	2.30	0.44
1:C:1920:DC:H2''	1:C:1921:DG:C8	2.53	0.44
2:D:1962:DC:C2'	2:D:1963:DG:C5'	2.96	0.44
3:A:430:ARG:HG2	3:A:438:LEU:HB3	2.00	0.44
3:A:415:HIS:CE1	3:A:492:GLU:HG3	2.52	0.44
3:A:375:LEU:HD21	3:A:516:ALA:HB1	1.99	0.44
3:A:35:GLN:CG	3:A:97:GLN:HG3	2.38	0.44
3:B:1346:PRO:HB3	3:B:1399:LEU:CD1	2.47	0.44
3:B:1477:THR:HG23	3:B:1478:LEU:H	1.82	0.44
3:B:1663:GLU:OE1	3:B:1696:HIS:CE1	2.71	0.44
3:A:213:GLY:O	3:A:218:ARG:HD3	2.18	0.43
3:B:1035:GLN:O	3:B:1110:ARG:NE	2.50	0.43
3:B:1581:ILE:HD11	3:B:1692:LEU:HD22	1.99	0.43
3:B:1693:PHE:C	3:B:1693:PHE:CD2	2.91	0.43
3:A:11:GLY:HA3	3:A:65:ASP:HB3	2.00	0.43
3:A:637:SER:OG	3:A:638:THR:N	2.51	0.43
3:A:574:MSE:HE1	3:A:691:THR:N	2.34	0.43
3:A:717:GLU:HA	3:A:722:LEU:HD23	2.00	0.43
3:A:379:LYS:HE2	3:A:383:GLU:OE2	2.17	0.43
3:B:1076:ARG:O	3:B:1078:PHE:N	2.52	0.43
3:A:191:LEU:HG	3:A:195:ARG:HH12	1.82	0.43
3:A:356:LEU:HD11	3:A:378:LEU:HD13	2.01	0.43
3:A:474:GLN:HG2	3:A:476:TYR:OH	2.18	0.43
3:A:448:TYR:CD1	3:A:485:GLU:HG3	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1015:PRO:HG2	3:B:1016:LEU:H	1.83	0.43
3:B:1748:PRO:HB2	3:B:1751:VAL:HG23	2.00	0.43
3:A:410:ALA:O	3:A:413:ALA:HB3	2.18	0.43
3:A:682:GLU:O	3:A:686:GLU:HG3	2.17	0.43
3:A:678:THR:HA	3:A:700:LEU:CD2	2.49	0.43
3:B:1167:TYR:CD2	3:B:1197:ARG:HD3	2.53	0.43
3:B:1435:ILE:HG23	3:B:1456:TYR:CD2	2.54	0.43
3:B:1454:ARG:HD3	3:B:1457:TYR:CE2	2.54	0.43
3:B:1574:MSE:HG2	3:B:1579:VAL:HG21	2.00	0.43
1:C:1901:DG:C1'	1:C:1902:DC:H5''	2.46	0.43
2:D:1955:DG:C2'	2:D:1956:DA:C8	3.01	0.43
3:A:320:GLU:O	3:A:324:ARG:HB2	2.19	0.43
3:B:1554:ARG:NH1	3:B:1554:ARG:HG2	2.33	0.43
3:B:1564:ARG:O	3:B:1565:THR:HG23	2.19	0.43
3:A:685:HIS:CE1	3:A:707:ARG:HB2	2.54	0.43
3:A:5:LEU:CD1	3:A:44:GLY:HA3	2.46	0.43
3:A:565:THR:CG2	3:A:566:GLU:N	2.81	0.43
3:B:1108:VAL:O	3:B:1108:VAL:HG12	2.17	0.43
3:B:1116:LEU:N	3:B:1116:LEU:HD12	2.34	0.43
3:B:1250:MSE:HB3	3:B:1295:PRO:HB2	2.01	0.43
3:B:1580:LEU:HD23	3:B:1693:PHE:HB3	2.00	0.43
3:A:581:ILE:HD13	3:A:592:PHE:HD2	1.84	0.43
3:B:1739:VAL:HG21	3:B:1759:LEU:HD11	2.01	0.43
3:A:42:CYS:O	3:A:47:ALA:HB2	2.18	0.42
3:A:750:GLU:CD	3:A:750:GLU:H	2.21	0.42
3:B:1122:LEU:HD21	3:B:1341:LEU:CD1	2.49	0.42
3:B:1141:ASP:N	7:B:70:HOH:O	2.49	0.42
3:B:1174:ARG:N	3:B:1175:PRO:HD3	2.34	0.42
3:B:1188:GLY:O	3:B:1192:ASP:OD1	2.36	0.42
3:B:1345:SER:CB	3:B:1392:LEU:HD22	2.48	0.42
3:B:1388:GLU:O	3:B:1389:ASP:HB2	2.19	0.42
3:A:143:TRP:CE3	3:A:166:LEU:HD22	2.54	0.42
3:A:267:ARG:O	3:A:269:GLN:N	2.52	0.42
3:A:348:ASP:O	3:A:351:ALA:HB3	2.20	0.42
3:B:1349:LEU:HB3	3:B:1386:LEU:HD11	2.01	0.42
3:B:1491:LEU:O	3:B:1495:ILE:HG13	2.20	0.42
3:A:535:GLU:HG3	3:A:539:ARG:NH1	2.34	0.42
3:A:12:PRO:HG2	3:A:65:ASP:OD2	2.18	0.42
3:A:54:LEU:HD13	3:A:81:TYR:CD1	2.54	0.42
3:B:1346:PRO:HD2	3:B:1392:LEU:HB2	2.00	0.42
2:D:1964:DC:H2''	2:D:1965:DT:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:99:GLU:HB2	3:A:109:ARG:NH2	2.34	0.42
3:A:145:LEU:HD22	3:A:146:ALA:N	2.34	0.42
3:A:250:MSE:HE2	3:A:619:PHE:HB2	2.01	0.42
3:A:751:VAL:HG21	3:B:1650:LEU:HD13	2.01	0.42
3:A:35:GLN:CB	3:A:96:ASP:HA	2.48	0.42
3:B:1099:GLU:HA	3:B:1100:PRO:HD2	1.76	0.42
3:B:1137:ILE:HA	3:B:1144:GLY:O	2.19	0.42
3:B:1354:ARG:NH1	3:B:1358:ILE:HD12	2.35	0.42
3:A:442:TYR:CG	3:A:443:ASN:N	2.87	0.42
3:B:1097:GLN:HE21	3:B:1110:ARG:NE	2.17	0.42
3:B:1470:LEU:HD22	3:B:1473:ARG:HE	1.85	0.42
3:B:1693:PHE:HD2	3:B:1693:PHE:C	2.22	0.42
3:A:396:GLU:O	3:A:397:GLY:O	2.37	0.42
3:B:1001:MSE:CB	3:B:1004:MSE:HB2	2.50	0.42
3:B:1742:ALA:O	3:B:1745:ALA:HB3	2.20	0.42
3:A:140:GLY:N	7:A:1919:HOH:O	2.22	0.42
3:A:752:VAL:O	3:A:755:ALA:HB3	2.20	0.42
3:B:1041:GLU:OE1	3:B:1072:GLY:HA3	2.19	0.42
3:B:1390:PRO:HA	3:B:1391:PRO:HD3	1.86	0.42
3:B:1678:THR:HA	3:B:1700:LEU:HD21	2.01	0.42
3:A:337:THR:OG1	3:A:518:ARG:NH2	2.53	0.42
3:A:449:TYR:CD1	3:A:449:TYR:C	2.93	0.42
3:B:1462:LYS:C	3:B:1464:TYR:N	2.71	0.42
3:B:1370:VAL:CG1	3:B:1523:ILE:HG21	2.50	0.42
3:B:1747:LEU:HD13	3:B:1748:PRO:CD	2.49	0.42
3:A:117:THR:OG1	3:A:120:THR:HG23	2.20	0.42
3:A:366:LEU:HD11	3:A:527:LEU:HD11	2.00	0.42
3:B:1217:LEU:HD23	3:B:1217:LEU:HA	1.75	0.42
3:B:1451:GLU:HG3	3:B:1475:ARG:HG2	2.01	0.42
1:C:1910:DG:H2"	1:C:1911:DC:OP2	2.20	0.42
3:A:747:LEU:HD22	3:A:748:PRO:HD2	2.01	0.41
3:A:40:TYR:OH	3:A:96:ASP:OD1	2.34	0.41
3:B:1013:LEU:CD2	3:B:1021:VAL:HG21	2.50	0.41
3:B:1024:ARG:HD2	3:B:1024:ARG:O	2.20	0.41
3:B:1232:GLN:CG	3:B:1232:GLN:O	2.68	0.41
3:B:1421:TYR:CD2	3:B:1421:TYR:C	2.93	0.41
3:B:1488:VAL:O	3:B:1492:GLU:HG3	2.19	0.41
3:A:347:LYS:HB2	3:A:347:LYS:HE2	1.87	0.41
3:A:394:VAL:CG1	3:A:395:SER:N	2.82	0.41
3:B:1167:TYR:CE2	3:B:1197:ARG:HD3	2.54	0.41
3:B:1625:ARG:NH1	7:B:8:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:387:VAL:HG23	3:A:389:ASP:C	2.40	0.41
3:A:387:VAL:O	3:A:390:PRO:HD3	2.19	0.41
3:A:450:LEU:HA	3:A:450:LEU:HD23	1.92	0.41
3:A:585:ASN:ND2	3:A:589:LYS:HZ1	2.18	0.41
3:B:1280:ARG:NH1	3:B:1323:ARG:O	2.53	0.41
3:B:1577:GLU:HB3	3:B:1707:ARG:O	2.20	0.41
3:B:1693:PHE:CE2	3:B:1695:THR:HB	2.55	0.41
3:A:339:LEU:HD23	3:A:344:ALA:CB	2.49	0.41
3:A:421:TYR:CD2	3:A:422:PHE:N	2.88	0.41
3:B:1013:LEU:HD12	3:B:1013:LEU:HA	1.76	0.41
3:B:1253:PRO:HB2	7:B:90:HOH:O	2.20	0.41
3:B:1438:LEU:HD13	3:B:1452:VAL:HG22	2.02	0.41
2:D:1969:DG:H2''	2:D:1970:DT:O5'	2.20	0.41
3:A:170:LEU:CD1	3:A:175:PRO:HG3	2.50	0.41
3:A:379:LYS:O	3:A:383:GLU:HG3	2.20	0.41
3:A:464:TYR:HB3	3:A:476:TYR:CD2	2.56	0.41
3:B:1429:GLU:O	3:B:1431:GLU:N	2.54	0.41
3:B:1508:GLU:O	3:B:1512:ARG:HG3	2.20	0.41
3:B:1636:LYS:HD3	3:B:1640:MSE:HE3	2.02	0.41
3:A:158:THR:OG1	3:A:159:VAL:N	2.53	0.41
3:A:273:PHE:HD1	3:A:292:LEU:CD1	2.34	0.41
3:B:1163:LYS:HG3	3:B:1167:TYR:CE1	2.56	0.41
3:B:1465:ARG:HH11	3:B:1465:ARG:HG3	1.86	0.41
3:B:1543:VAL:CG1	3:B:1544:ARG:N	2.84	0.41
3:B:1684:LEU:HA	3:B:1684:LEU:HD23	1.94	0.41
3:B:1708:LEU:HD12	3:B:1709:LYS:N	2.31	0.41
3:A:167:TYR:HD2	3:A:197:ARG:NH1	2.19	0.41
3:A:376:SER:N	3:A:377:PRO:CD	2.82	0.41
3:A:712:HIS:CE1	3:A:729:LEU:HB2	2.56	0.41
3:A:765:ARG:NH1	3:A:765:ARG:HG2	2.32	0.41
3:A:51:ALA:O	3:A:55:GLY:N	2.54	0.41
3:A:564:ARG:HH11	3:A:564:ARG:HG2	1.86	0.41
3:A:682:GLU:O	3:A:685:HIS:HB3	2.20	0.41
3:B:1256:THR:CG2	3:B:1260:LEU:HD22	2.51	0.41
3:B:1449:TYR:CD1	3:B:1449:TYR:C	2.94	0.41
3:A:589:LYS:HZ2	3:A:696:HIS:CE1	2.39	0.41
3:A:722:LEU:HB2	3:A:744:MSE:CE	2.43	0.41
3:B:1099:GLU:O	3:B:1100:PRO:C	2.59	0.41
3:B:1225:LEU:O	3:B:1229:GLN:HG3	2.21	0.41
3:B:1400:ILE:HG12	3:B:1499:GLU:HG3	2.03	0.41
3:B:1564:ARG:HB2	3:B:1564:ARG:HE	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:394:VAL:HG13	3:A:395:SER:H	1.83	0.41
3:A:482:LYS:CD	3:A:486:ARG:HH22	2.34	0.41
3:A:519:GLU:O	3:A:519:GLU:HG2	2.20	0.41
3:A:52:ARG:CG	3:A:53:ALA:N	2.84	0.41
3:A:669:SER:HB2	3:B:1736:SER:OG	2.21	0.41
3:B:1049:ARG:NH1	3:B:1049:ARG:HG3	2.36	0.41
3:B:1170:LEU:HA	3:B:1170:LEU:HD22	1.85	0.41
3:B:1269:GLN:HG3	3:B:1270:ASP:N	2.35	0.41
3:B:1429:GLU:C	3:B:1431:GLU:H	2.24	0.41
2:D:1971:DC:C2'	2:D:1972:DG:H5''	2.50	0.41
2:D:1970:DT:H2''	2:D:1971:DC:C6	2.56	0.41
3:A:491:LEU:O	3:A:495:ILE:HG13	2.21	0.40
3:A:639:PHE:O	3:A:643:MSE:HG2	2.21	0.40
3:B:1174:ARG:NH2	3:B:1264:GLU:OE1	2.55	0.40
3:B:1609:VAL:HB	3:B:1610:PRO:HD2	2.03	0.40
3:A:468:GLN:HE22	3:A:475:ARG:HH11	1.68	0.40
3:A:554:ARG:O	3:A:555:ALA:CB	2.69	0.40
3:A:306:LEU:HD23	3:A:606:GLY:O	2.21	0.40
3:B:1148:LEU:HB2	3:B:1224:LEU:HD13	2.03	0.40
2:D:1957:DG:H2''	2:D:1958:DC:C5	2.56	0.40
2:D:1956:DA:H2''	2:D:1957:DG:H8	1.86	0.40
1:C:1916:DG:N2	2:D:1960:DG:N2	2.69	0.40
3:A:170:LEU:HD11	3:A:175:PRO:HG3	2.03	0.40
3:A:214:PRO:O	3:A:218:ARG:HG3	2.22	0.40
3:A:301:PRO:O	3:A:304:ALA:HB3	2.21	0.40
3:A:722:LEU:HD11	3:A:737:TYR:HD2	1.85	0.40
3:B:1068:THR:OG1	3:B:1069:PRO:HD2	2.20	0.40
3:B:1143:TRP:CZ3	3:B:1161:LYS:O	2.69	0.40
3:B:1210:GLU:OE1	3:B:1221:ARG:CD	2.69	0.40
3:B:1421:TYR:C	3:B:1423:LEU:H	2.23	0.40
3:B:1385:ALA:HB2	3:B:1404:TYR:CZ	2.57	0.40
3:A:218:ARG:NE	7:A:1886:HOH:O	2.54	0.40
3:A:228:ALA:HB3	3:A:236:LEU:HD11	2.04	0.40
3:A:748:PRO:HB2	3:A:751:VAL:CG2	2.50	0.40
3:B:1263:PHE:O	3:B:1271:THR:HG21	2.21	0.40
3:B:1558:HIS:HD2	3:B:1561:VAL:H	1.68	0.40
1:C:1918:DC:H2''	1:C:1919:DT:C5'	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
3	A	755/768 (98%)	688 (91%)	58 (8%)	9 (1%)	15	37
3	B	743/768 (97%)	661 (89%)	65 (9%)	17 (2%)	7	19
All	All	1498/1536 (98%)	1349 (90%)	123 (8%)	26 (2%)	11	27

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	1010	PRO
3	B	1011	GLY
3	B	1233	GLY
3	B	1269	GLN
3	B	1391	PRO
3	B	1396	GLU
3	A	141	ASP
3	A	187	ASN
3	A	268	GLY
3	A	397	GLY
3	A	719	ALA
3	B	1077	ALA
3	A	3	GLY
3	A	98	VAL
3	A	703	LEU
3	B	1315	GLU
3	B	1438	LEU
3	A	10	PRO
3	B	1078	PHE
3	B	1389	ASP
3	B	1267	ARG
3	B	1388	GLU
3	B	1719	ALA
3	B	1209	PRO
3	B	1435	ILE

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Mol	Chain	Res	Type
3	B	1394	VAL

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	
3	A	613/606 (101%)	572 (93%)	41 (7%)	19	42
3	B	608/606 (100%)	565 (93%)	43 (7%)	17	39
All	All	1221/1212 (101%)	1137 (93%)	84 (7%)	18	41

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	MSE
3	A	18	GLN
3	A	35	GLN
3	A	58	LEU
3	A	60	HIS
3	A	66	PHE
3	A	99	GLU
3	A	112	VAL
3	A	145	LEU
3	A	161	LYS
3	A	174	ARG
3	A	195	ARG
3	A	196	LYS
3	A	215	LEU
3	A	243	PHE
3	A	260	LEU
3	A	274	SER
3	A	276	LEU
3	A	308	ARG
3	A	335	LEU
3	A	363	ARG
3	A	378	LEU

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Mol	Chain	Res	Type
3	A	509	ARG
3	A	527	LEU
3	A	554	ARG
3	A	557	ARG
3	A	563	ARG
3	A	578	LEU
3	A	605	VAL
3	A	607	SER
3	A	625	ARG
3	A	636	LYS
3	A	660	LEU
3	A	666	ARG
3	A	672	ASP
3	A	674	VAL
3	A	693	PHE
3	A	699	GLU
3	A	716	ARG
3	A	735	LYS
3	A	747	LEU
3	B	1002	GLU
3	B	1006	LYS
3	B	1013	LEU
3	B	1018	GLN
3	B	1030	TYR
3	B	1070	MSE
3	B	1075	LEU
3	B	1115	LEU
3	B	1117	THR
3	B	1122	LEU
3	B	1123	GLN
3	B	1145	LEU
3	B	1161	LYS
3	B	1170	LEU
3	B	1183	GLU
3	B	1192	ASP
3	B	1217	LEU
3	B	1238	LEU
3	B	1250	MSE
3	B	1260	LEU
3	B	1276	LEU
3	B	1315	GLU
3	B	1332	LEU

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Mol	Chain	Res	Type
3	B	1353	ARG
3	B	1358	ILE
3	B	1378	LEU
3	B	1391	PRO
3	B	1396	GLU
3	B	1416	ARG
3	B	1446	PHE
3	B	1454	ARG
3	B	1473	ARG
3	B	1484	LYS
3	B	1505	GLU
3	B	1546	ARG
3	B	1557	ARG
3	B	1563	ARG
3	B	1605	VAL
3	B	1648	LEU
3	B	1663	GLU
3	B	1693	PHE
3	B	1727	GLN
3	B	1747	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	35	GLN
3	A	60	HIS
3	A	114	GLN
3	A	132	ASN
3	A	173	HIS
3	A	232	GLN
3	A	239	GLN
3	A	269	GLN
3	A	357	GLN
3	A	415	HIS
3	A	468	GLN
3	A	585	ASN
3	A	685	HIS
3	B	1097	GLN
3	B	1114	GLN
3	B	1123	GLN
3	B	1173	HIS
3	B	1269	GLN

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Mol	Chain	Res	Type
3	B	1289	GLN
3	B	1415	HIS
3	B	1474	GLN
3	B	1558	HIS
3	B	1585	ASN
3	B	1604	GLN
3	B	1685	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
5	SO4	A	1853	-	4,4,4	0.37	0	6,6,6	0.05	0
5	SO4	A	852	-	4,4,4	0.26	0	6,6,6	0.25	0
6	ADP	A	999	4	25,29,29	1.07	2 (8%)	24,45,45	2.05	6 (25%)
5	SO4	B	1852	-	4,4,4	0.31	0	6,6,6	0.33	0
6	ADP	B	1999	4	25,29,29	0.99	2 (8%)	24,45,45	1.58	5 (20%)
5	SO4	B	853	-	4,4,4	0.33	0	6,6,6	0.14	0

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
5	SO4	A	1853	-	-	0/0/0/0	0/0/0/0
5	SO4	A	852	-	-	0/0/0/0	0/0/0/0
6	ADP	A	999	4	-	0/12/32/32	0/3/3/3
5	SO4	B	1852	-	-	0/0/0/0	0/0/0/0
6	ADP	B	1999	4	-	0/12/32/32	0/3/3/3
5	SO4	B	853	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	999	ADP	C8-N7	-2.16	1.30	1.34
6	B	1999	ADP	C8-N7	-2.10	1.30	1.34
6	B	1999	ADP	C2-N3	2.01	1.35	1.32
6	A	999	ADP	C2-N3	2.25	1.35	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	999	ADP	C5'-C4'-C3'	-4.78	97.07	115.29
6	B	1999	ADP	N3-C2-N1	-4.58	124.87	128.86
6	A	999	ADP	N3-C2-N1	-3.84	125.51	128.86
6	B	1999	ADP	O4'-C4'-C5'	-2.68	100.34	109.40
6	B	1999	ADP	O2B-PB-O1B	2.09	118.67	110.50
6	A	999	ADP	C4-C5-N7	2.09	111.43	109.41
6	A	999	ADP	C2'-C3'-C4'	2.37	107.24	102.62
6	B	1999	ADP	O3'-C3'-C4'	2.53	118.47	111.09
6	B	1999	ADP	C4-C5-N7	3.15	112.45	109.41
6	A	999	ADP	O2B-PB-O1B	3.21	123.07	110.50
6	A	999	ADP	O5'-C5'-C4'	5.30	127.81	109.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	999	ADP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1999	ADP	3	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.