



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:08 PM GMT

PDB ID : 5EAX  
Title : Crystal structure of Dna2 in complex with an ssDNA  
Authors : Zhou, C.; Pourmal, S.; Pavletich, N.P.  
Deposited on : 2015-10-17  
Resolution : 3.05 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

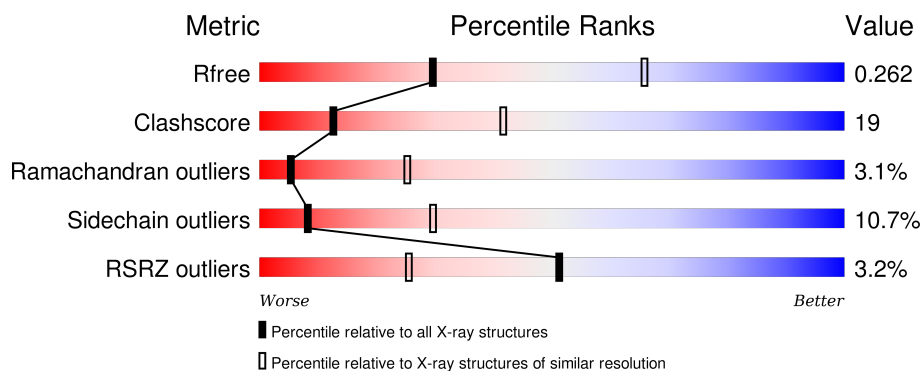
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

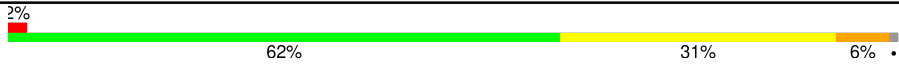

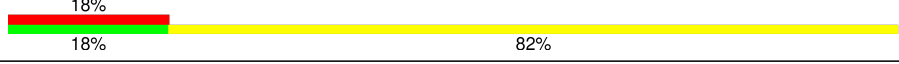

The reported resolution of this entry is 3.05 Å.

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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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  $\geq 3$ , 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	1056	
1	B	1056	
2	E	17	
2	H	17	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17280 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 replication ATP-dependent helicase/nuclease DNA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1046	Total	C	N	O	S	0	0	0
			8268	5221	1456	1546	45			
1	B	1046	Total	C	N	O	S	0	0	0
			8268	5221	1456	1546	45			

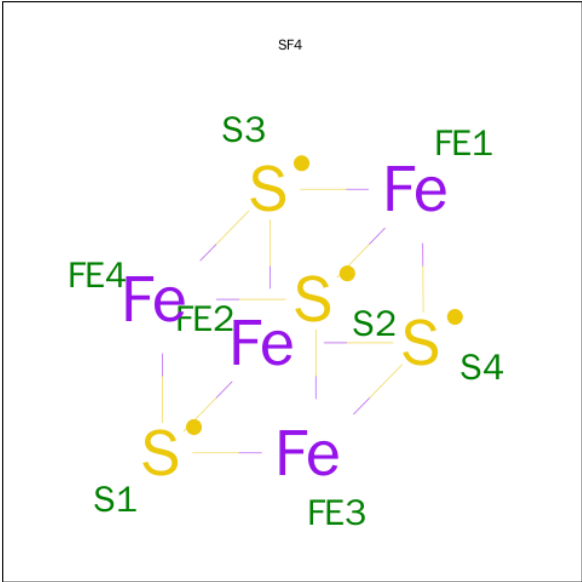
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	ALA	ASP	engineered mutation	UNP Q6ZQJ5
B	278	ALA	ASP	engineered mutation	UNP Q6ZQJ5

- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*T)-3').

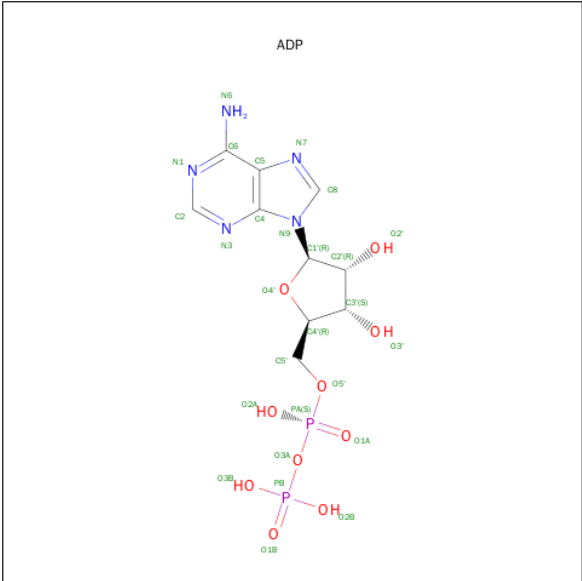
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	P	0	0	0
			337	170	34	117	16			
2	H	17	Total	C	N	O	P	0	0	0
			337	170	34	117	16			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

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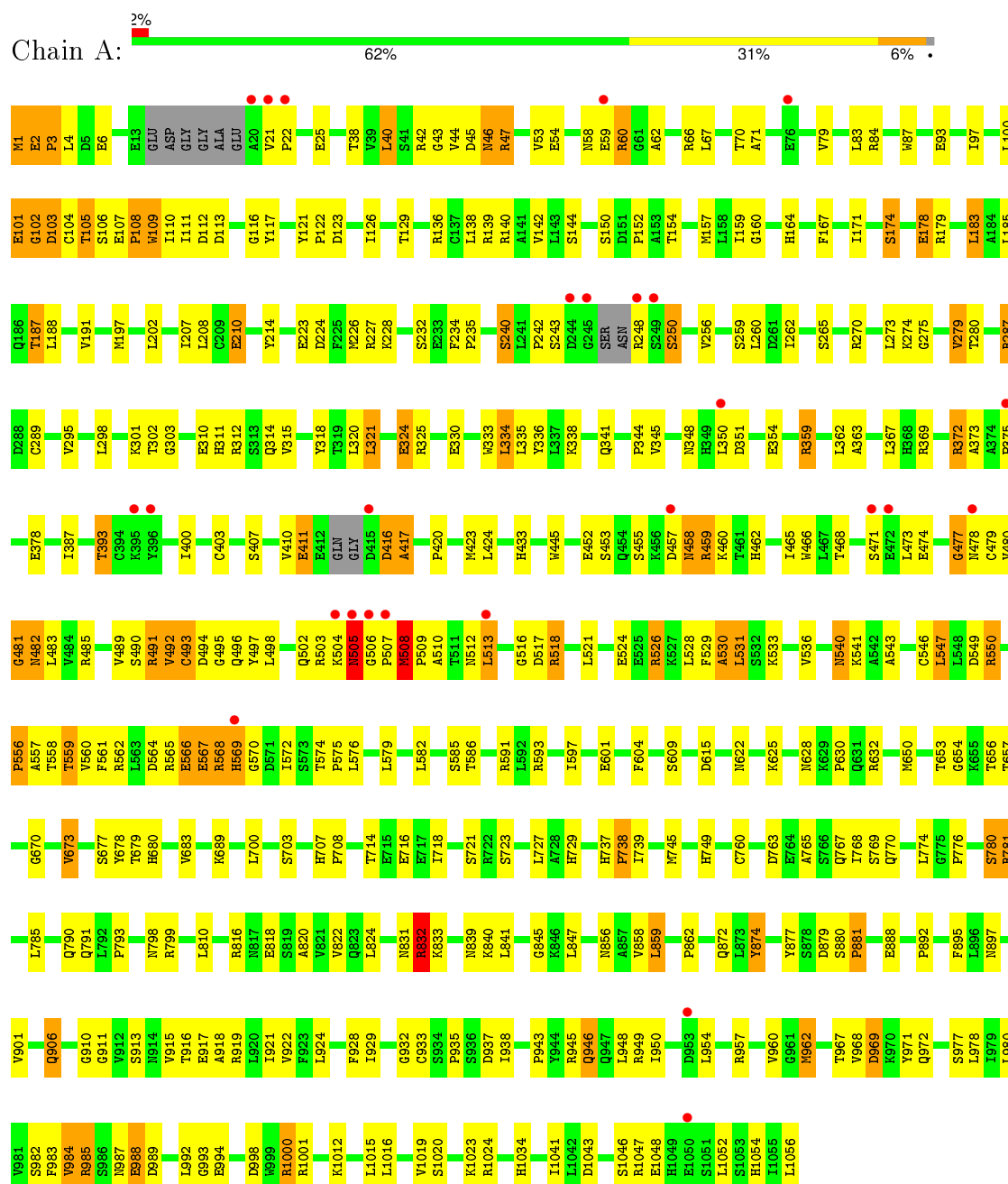
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

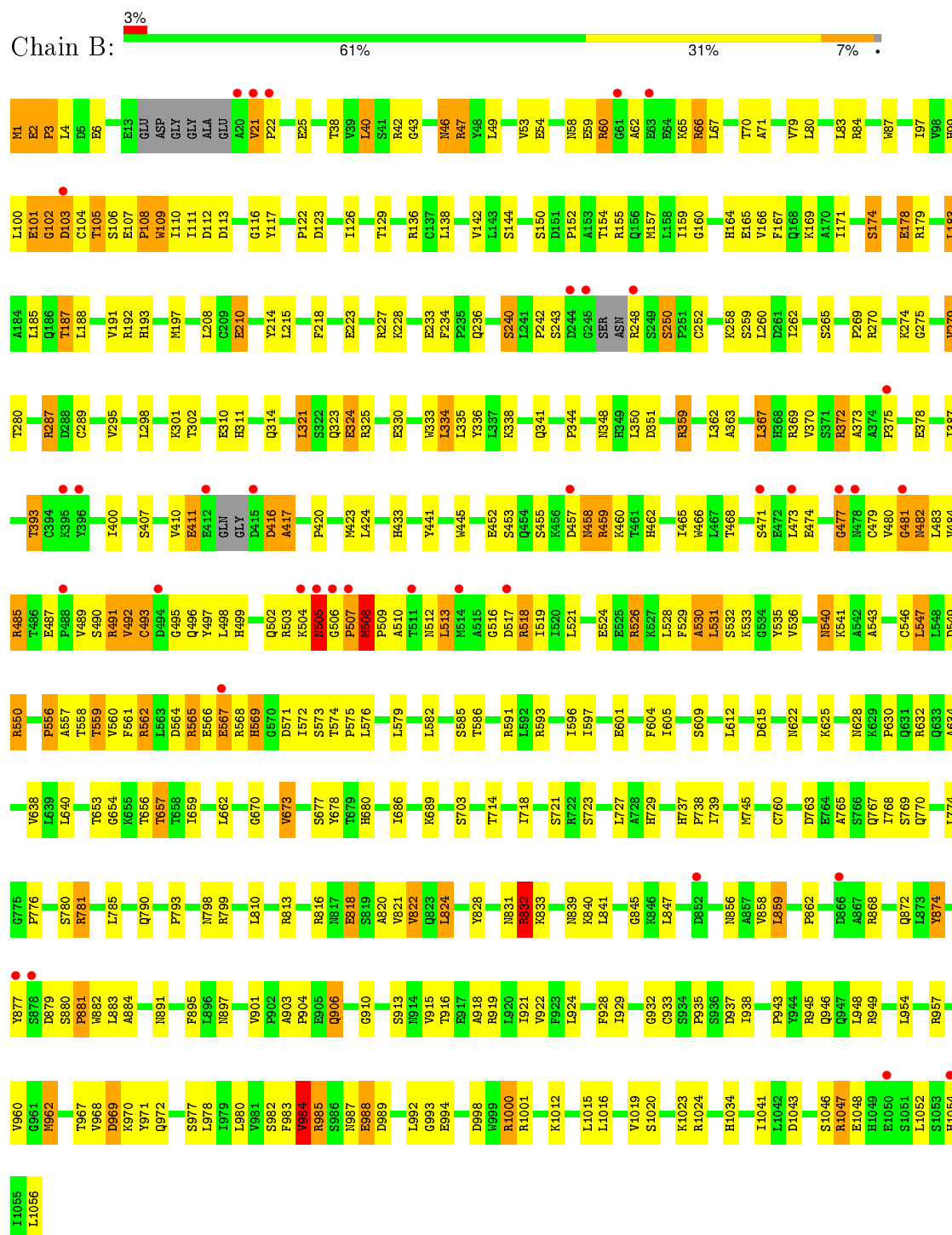
### 3 Residue-property plots

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

- Molecule 1: DNA replication ATP-dependent helicase/nuclease DNA2



- Molecule 1: DNA replication ATP-dependent helicase/nuclease DNA2

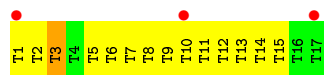


- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP)-3')



- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*T)-3')

Chain H:  18% 18% 76% 6%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.23Å 149.21Å 172.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.05 29.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	87.4 (29.99-3.05) 84.7 (29.97-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.223 , 0.256 0.227 , 0.262	Depositor DCC
$R_{free}$ test set	1466 reflections (2.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 68665 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.05 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3881e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SF4, 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	0.49	0/8418	0.71	2/11383 (0.0%)
1	B	0.48	0/8418	0.70	2/11383 (0.0%)
2	E	0.48	0/370	0.86	0/570
2	H	0.50	1/370 (0.3%)	0.84	0/570
All	All	0.48	1/17576 (0.0%)	0.71	4/23906 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	3	DT	O3'-P	-5.46	1.54	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LEU	CA-CB-CG	6.28	129.74	115.30
1	B	4	LEU	CA-CB-CG	6.25	129.67	115.30
1	A	482	ASN	CB-CA-C	5.25	120.90	110.40
1	B	482	ASN	CB-CA-C	5.20	120.79	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	481	GLY	Peptide
1	A	508	MET	Peptide
1	B	481	GLY	Peptide
1	B	507	PRO	Peptide
1	B	508	MET	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8268	0	8412	303	0
1	B	8268	0	8412	313	0
2	E	337	0	206	46	0
2	H	337	0	206	42	0
3	A	8	0	0	0	0
3	B	8	0	0	1	0
4	A	27	0	12	2	0
4	B	27	0	12	1	0
All	All	17280	0	17260	669	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 19.

All (669) 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:495:GLY:O	1:B:549:ASP:HA	1.34	1.26
1:A:495:GLY:O	1:A:549:ASP:HA	1.37	1.17
2:H:13:DT:H2''	2:H:14:DT:C5'	1.79	1.13
2:E:13:DT:H2''	2:E:14:DT:C5'	1.77	1.12
2:H:13:DT:C2'	2:H:14:DT:H5''	1.84	1.08
1:B:43:GLY:H	1:B:105:THR:HG21	1.15	1.07
2:E:13:DT:C2'	2:E:14:DT:H5''	1.82	1.06
1:A:43:GLY:H	1:A:105:THR:HG21	1.14	1.05
1:A:988:GLU:HG2	1:A:989:ASP:H	1.22	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:ARG:HG2	1:B:526:ARG:HH11	1.25	1.01
1:B:988:GLU:HG2	1:B:989:ASP:H	1.23	1.00
1:B:458:ASN:HB2	1:B:569:HIS:HB3	1.45	0.98
1:B:102:GLY:HA3	1:B:117:TYR:H	1.29	0.98
1:B:102:GLY:CA	1:B:117:TYR:H	1.78	0.97
1:A:102:GLY:HA3	1:A:117:TYR:H	1.29	0.95
1:A:102:GLY:CA	1:A:117:TYR:H	1.80	0.95
1:A:458:ASN:HB2	1:A:569:HIS:HB3	1.49	0.94
1:A:526:ARG:HG2	1:A:526:ARG:HH11	1.30	0.94
1:A:910:GLY:HA2	2:E:3:DT:H72	1.48	0.93
2:E:2:DT:H2"	2:E:3:DT:OP2	1.67	0.92
2:H:2:DT:H2"	2:H:3:DT:OP2	1.67	0.92
1:A:654:GLY:HA2	4:A:1102:ADP:O2B	1.67	0.92
1:B:654:GLY:HA2	4:B:1102:ADP:O2B	1.72	0.90
1:A:799:ARG:HH22	1:A:994:GLU:HG3	1.37	0.90
1:B:465:ILE:HA	1:B:562:ARG:NH1	1.92	0.85
1:B:799:ARG:HH22	1:B:994:GLU:HG3	1.41	0.84
1:A:101:GLU:C	1:A:103:ASP:H	1.80	0.82
1:B:43:GLY:N	1:B:105:THR:HG21	1.93	0.82
2:H:13:DT:H2"	2:H:14:DT:H5"	0.88	0.82
1:A:43:GLY:N	1:A:105:THR:HG21	1.93	0.82
1:A:2:GLU:HB2	1:A:3:PRO:HD3	1.61	0.81
1:B:2:GLU:HB2	1:B:3:PRO:HD3	1.61	0.81
1:A:678:TYR:OH	2:E:6:DT:O2	1.99	0.80
1:A:459:ARG:HG2	1:A:459:ARG:HH11	1.46	0.79
1:B:160:GLY:HA2	1:B:302:THR:HG21	1.63	0.79
2:H:8:DT:H2"	2:H:9:DT:H5"	1.63	0.79
1:B:526:ARG:NH1	1:B:526:ARG:HG2	1.92	0.79
1:B:498:LEU:HA	1:B:547:LEU:CD2	2.13	0.79
1:A:160:GLY:HA2	1:A:302:THR:HG21	1.65	0.78
1:A:799:ARG:NH2	1:A:994:GLU:HG3	1.98	0.78
1:B:101:GLU:C	1:B:103:ASP:H	1.82	0.78
1:B:275:GLY:HA3	1:B:321:LEU:HD21	1.65	0.78
1:A:498:LEU:HA	1:A:547:LEU:CD2	2.13	0.77
1:A:533:LYS:NZ	2:E:11:DT:H5'	1.98	0.77
1:A:465:ILE:HA	1:A:562:ARG:NH1	2.00	0.77
2:H:2:DT:C2	2:H:3:DT:H72	2.19	0.77
1:B:459:ARG:HH11	1:B:459:ARG:HG2	1.49	0.76
2:E:8:DT:H2"	2:E:9:DT:H5"	1.67	0.76
1:B:129:THR:HG21	2:H:13:DT:H3'	1.68	0.75
1:B:656:THR:HG22	1:B:689:LYS:HE3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLY:HA3	1:A:321:LEU:HD21	1.69	0.75
2:E:13:DT:H2''	2:E:14:DT:H5''	0.86	0.74
1:B:102:GLY:HA3	1:B:117:TYR:N	2.01	0.74
1:A:260:LEU:HD11	1:A:295:VAL:HG22	1.70	0.73
2:E:11:DT:OP1	2:E:12:DT:C2	2.42	0.73
1:B:572:ILE:HD12	1:B:576:LEU:HD11	1.70	0.73
1:A:988:GLU:HG2	1:A:989:ASP:N	2.01	0.73
2:H:12:DT:H1'	2:H:13:DT:H5''	1.70	0.73
1:A:526:ARG:HG2	1:A:526:ARG:NH1	1.97	0.73
1:A:921:ILE:HG23	1:A:1016:LEU:HD22	1.71	0.73
2:E:2:DT:C2	2:E:3:DT:H73	2.23	0.72
1:A:656:THR:HG22	1:A:689:LYS:HE3	1.70	0.72
1:A:102:GLY:HA3	1:A:117:TYR:N	2.03	0.72
1:A:880:SER:N	1:A:881:PRO:HD2	2.04	0.72
2:E:12:DT:H1'	2:E:13:DT:H5''	1.72	0.72
1:B:880:SER:N	1:B:881:PRO:HD2	2.05	0.72
1:B:465:ILE:HA	1:B:562:ARG:HH11	1.55	0.72
1:B:178:GLU:H	1:B:178:GLU:CD	1.94	0.71
2:H:8:DT:H2''	2:H:9:DT:C5'	2.20	0.71
1:B:799:ARG:NH2	1:B:994:GLU:HG3	2.04	0.71
1:A:477:GLY:O	1:A:512:ASN:HB2	1.91	0.71
2:H:11:DT:OP1	2:H:12:DT:C2	2.43	0.70
1:B:988:GLU:HG2	1:B:989:ASP:N	2.03	0.70
1:A:498:LEU:HA	1:A:547:LEU:HD22	1.71	0.70
1:A:227:ARG:HG2	1:A:234:PHE:CE1	2.26	0.70
1:A:745:MET:HB2	2:E:8:DT:H5'	1.73	0.69
1:A:2:GLU:HB2	1:A:3:PRO:CD	2.22	0.69
1:B:453:SER:HB2	1:B:572:ILE:HG21	1.73	0.69
1:B:498:LEU:HA	1:B:547:LEU:HD22	1.72	0.69
1:B:274:LYS:HE3	2:H:12:DT:OP2	1.92	0.69
1:B:287:ARG:HG3	1:B:287:ARG:HH11	1.58	0.69
1:A:985:ARG:NH1	1:A:993:GLY:H	1.91	0.69
1:B:516:GLY:H	1:B:536:VAL:HB	1.57	0.69
1:B:477:GLY:O	1:B:512:ASN:HB2	1.93	0.69
1:B:745:MET:HB2	2:H:8:DT:H5'	1.75	0.68
1:A:799:ARG:HH22	1:A:994:GLU:CG	2.06	0.68
1:A:107:GLU:HG2	1:A:109:TRP:HZ3	1.58	0.68
1:B:107:GLU:HG2	1:B:109:TRP:HZ3	1.58	0.68
1:B:2:GLU:HB2	1:B:3:PRO:CD	2.23	0.68
1:A:46:ASN:H	1:A:46:ASN:HD22	1.40	0.68
1:A:840:LYS:HD2	1:A:1034:HIS:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:SER:O	1:B:411:GLU:HB3	1.94	0.68
1:B:1:MET:N	1:B:1:MET:SD	2.58	0.68
2:E:8:DT:H2''	2:E:9:DT:C5'	2.24	0.67
1:B:533:LYS:NZ	2:H:11:DT:H5'	2.09	0.67
1:B:458:ASN:HB2	1:B:569:HIS:CB	2.22	0.67
1:A:516:GLY:H	1:A:536:VAL:HB	1.59	0.67
1:A:453:SER:HB2	1:A:572:ILE:HG21	1.77	0.67
1:B:459:ARG:HH11	1:B:459:ARG:CG	2.08	0.67
1:B:840:LYS:HD2	1:B:1034:HIS:CD2	2.30	0.67
1:A:459:ARG:HH11	1:A:459:ARG:CG	2.08	0.66
2:H:5:DT:H2''	2:H:6:DT:OP2	1.95	0.66
1:B:287:ARG:HG3	1:B:287:ARG:NH1	2.10	0.66
1:A:533:LYS:HZ3	2:E:11:DT:H5'	1.61	0.66
1:A:528:LEU:O	1:A:531:LEU:HD12	1.96	0.66
1:B:790:GLN:O	1:B:1000:ARG:HG3	1.96	0.66
1:A:129:THR:HG21	2:E:13:DT:H3'	1.76	0.66
1:A:407:SER:O	1:A:411:GLU:HB3	1.96	0.65
1:B:260:LEU:HD11	1:B:295:VAL:HG22	1.77	0.65
1:A:101:GLU:C	1:A:103:ASP:N	2.50	0.65
1:A:493:CYS:O	1:A:496:GLN:HG2	1.96	0.65
1:B:59:GLU:O	1:B:60:ARG:HB2	1.94	0.65
1:A:59:GLU:O	1:A:60:ARG:HB2	1.95	0.65
1:B:493:CYS:O	1:B:496:GLN:HG2	1.96	0.65
1:A:510:ALA:HA	1:A:513:LEU:HD11	1.78	0.65
1:B:46:ASN:HD22	1:B:46:ASN:H	1.44	0.65
1:A:178:GLU:H	1:A:178:GLU:CD	1.99	0.65
1:A:680:HIS:NE2	2:E:8:DT:OP1	2.30	0.65
1:B:510:ALA:HA	1:B:513:LEU:HD11	1.79	0.65
1:B:528:LEU:O	1:B:531:LEU:HD12	1.97	0.64
1:A:1:MET:SD	1:A:1:MET:N	2.60	0.64
1:B:910:GLY:HA2	2:H:3:DT:C7	2.27	0.64
1:A:504:LYS:O	1:A:505:ASN:HB3	1.96	0.64
1:B:53:VAL:HG22	1:B:67:LEU:HD22	1.80	0.64
1:B:508:MET:SD	1:B:509:PRO:HD3	2.38	0.64
1:A:458:ASN:HB2	1:A:569:HIS:CB	2.26	0.64
1:B:468:THR:O	1:B:562:ARG:NH2	2.30	0.64
1:A:919:ARG:HD2	1:A:1056:LEU:HD23	1.79	0.64
1:B:138:LEU:O	1:B:142:VAL:HG23	1.98	0.64
1:B:104:CYS:O	1:B:105:THR:HB	1.98	0.64
1:B:985:ARG:NH1	1:B:993:GLY:H	1.95	0.63
1:A:104:CYS:O	1:A:105:THR:HB	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLU:OE1	1:A:526:ARG:NH2	2.32	0.63
1:A:287:ARG:HG3	1:A:287:ARG:HH11	1.63	0.63
1:B:504:LYS:O	1:B:505:ASN:HB3	1.96	0.63
1:B:79:VAL:HG11	1:B:108:PRO:HG2	1.80	0.63
1:B:799:ARG:HH22	1:B:994:GLU:CG	2.09	0.63
1:B:540:ASN:O	1:B:543:ALA:O	2.16	0.63
2:E:11:DT:OP1	2:E:12:DT:N3	2.32	0.63
1:B:324:GLU:OE1	1:B:526:ARG:NH2	2.31	0.63
1:A:468:THR:O	1:A:562:ARG:NH2	2.31	0.63
1:A:107:GLU:HG2	1:A:109:TRP:CZ3	2.34	0.63
1:A:53:VAL:HG22	1:A:67:LEU:HD22	1.80	0.63
1:B:458:ASN:CB	1:B:569:HIS:HB3	2.27	0.63
1:A:983:PHE:O	1:A:985:ARG:N	2.32	0.62
1:B:433:HIS:CE1	1:B:585:SER:HB3	2.34	0.62
1:B:897:ASN:HB3	1:B:1043:ASP:HA	1.81	0.62
1:A:507:PRO:O	1:A:508:MET:HB2	1.99	0.62
1:A:480:VAL:HG21	1:A:513:LEU:HD13	1.82	0.62
1:B:183:LEU:O	1:B:187:THR:HG23	2.00	0.62
1:B:227:ARG:HG2	1:B:234:PHE:CE1	2.35	0.62
1:B:101:GLU:C	1:B:103:ASP:N	2.53	0.62
1:B:673:VAL:HG13	1:B:739:ILE:HG12	1.80	0.62
1:B:556:PRO:O	1:B:558:THR:N	2.29	0.62
1:B:459:ARG:HH11	1:B:459:ARG:HA	1.64	0.62
1:A:250:SER:O	1:A:287:ARG:NH2	2.32	0.61
2:E:5:DT:H2"	2:E:6:DT:OP2	1.98	0.61
1:B:480:VAL:HG21	1:B:513:LEU:HD13	1.82	0.61
1:B:107:GLU:HG2	1:B:109:TRP:CZ3	2.35	0.61
2:E:10:DT:H2"	2:E:11:DT:OP2	1.99	0.61
1:B:262:ILE:HG22	1:B:279:VAL:HG13	1.83	0.61
1:B:106:SER:O	1:B:107:GLU:HG3	2.01	0.61
1:A:556:PRO:O	1:A:558:THR:N	2.28	0.61
1:B:274:LYS:CE	2:H:12:DT:OP2	2.49	0.61
1:A:508:MET:SD	1:A:509:PRO:HD3	2.41	0.61
1:A:895:PHE:HB3	1:A:1041:ILE:HG22	1.83	0.61
2:H:11:DT:OP1	2:H:12:DT:N3	2.34	0.61
1:B:126:ILE:HD11	1:B:363:ALA:HA	1.82	0.61
1:A:478:ASN:HB3	1:A:565:ARG:HG3	1.82	0.60
1:B:21:VAL:H	1:B:22:PRO:HD2	1.66	0.60
1:A:298:LEU:HD11	1:A:335:LEU:HB2	1.82	0.60
1:A:540:ASN:O	1:A:543:ALA:O	2.19	0.60
1:B:455:SER:O	1:B:458:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:PRO:O	1:B:508:MET:HB2	2.00	0.60
1:A:465:ILE:HA	1:A:562:ARG:HH11	1.66	0.60
1:B:250:SER:O	1:B:287:ARG:NH2	2.34	0.60
1:A:126:ILE:HG21	1:A:362:LEU:HD23	1.84	0.60
1:A:922:VAL:HG21	1:A:954:LEU:HB2	1.83	0.59
1:A:459:ARG:HA	1:A:459:ARG:HH11	1.66	0.59
1:A:767:GLN:OE1	1:A:972:GLN:NE2	2.34	0.59
1:B:2:GLU:N	1:B:6:GLU:HG3	2.17	0.59
1:B:445:TRP:HB3	1:B:579:LEU:HD11	1.84	0.59
1:A:872:GLN:NE2	1:A:877:TYR:HB2	2.17	0.59
1:B:839:ASN:ND2	1:B:847:LEU:HB2	2.17	0.59
1:A:46:ASN:H	1:A:46:ASN:ND2	2.00	0.59
1:B:335:LEU:O	1:B:336:TYR:HB2	2.02	0.59
1:A:445:TRP:HB3	1:A:579:LEU:HD11	1.83	0.59
1:B:922:VAL:HG21	1:B:954:LEU:HB2	1.84	0.59
1:B:767:GLN:OE1	1:B:972:GLN:NE2	2.35	0.59
1:A:242:PRO:HG2	1:A:330:GLU:OE2	2.03	0.59
1:B:510:ALA:HB3	1:B:541:LYS:HE2	1.84	0.59
1:B:335:LEU:O	1:B:341:GLN:O	2.21	0.59
1:A:262:ILE:HG22	1:A:279:VAL:HG13	1.84	0.59
1:B:460:LYS:HE3	1:B:567:GLU:HG3	1.83	0.59
1:B:566:GLU:O	1:B:567:GLU:HB2	2.03	0.59
1:B:872:GLN:NE2	1:B:877:TYR:HB2	2.18	0.59
1:B:992:LEU:HD13	1:B:1024:ARG:NH1	2.18	0.58
2:H:10:DT:H2"	2:H:11:DT:OP2	2.01	0.58
1:A:260:LEU:CD1	1:A:295:VAL:HG22	2.33	0.58
1:A:126:ILE:HD11	1:A:363:ALA:HA	1.83	0.58
2:H:8:DT:C2'	2:H:9:DT:H5"	2.33	0.58
1:A:572:ILE:HD12	1:A:576:LEU:HD11	1.83	0.58
1:A:335:LEU:O	1:A:336:TYR:HB2	2.03	0.58
1:A:106:SER:O	1:A:107:GLU:HG3	2.03	0.58
1:B:895:PHE:HB3	1:B:1041:ILE:HG22	1.83	0.58
1:B:919:ARG:HD2	1:B:1056:LEU:HD23	1.85	0.58
1:B:526:ARG:CG	1:B:526:ARG:HH11	2.10	0.58
1:A:859:LEU:HD12	1:A:1012:LYS:HD2	1.85	0.58
1:A:565:ARG:O	1:A:566:GLU:HG3	2.04	0.58
1:A:287:ARG:HG3	1:A:287:ARG:NH1	2.16	0.58
1:B:126:ILE:HG21	1:B:362:LEU:HD23	1.86	0.58
1:A:793:PRO:HG3	1:A:1000:ARG:NH2	2.19	0.57
1:B:945:ARG:NH1	2:H:5:DT:OP1	2.37	0.57
1:B:680:HIS:NE2	2:H:8:DT:OP1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ASN:HB2	1:B:351:ASP:OD2	2.04	0.57
1:A:433:HIS:CE1	1:A:585:SER:HB3	2.39	0.57
1:A:58:ASN:O	1:A:62:ALA:HB3	2.05	0.57
1:A:2:GLU:N	1:A:6:GLU:HG3	2.19	0.57
1:B:628:ASN:OD1	1:B:630:PRO:HD2	2.05	0.57
1:A:455:SER:O	1:A:458:ASN:ND2	2.37	0.57
1:A:840:LYS:HD2	1:A:1034:HIS:HD2	1.70	0.57
1:A:348:ASN:HB2	1:A:351:ASP:OD2	2.05	0.57
1:A:593:ARG:HG2	1:A:597:ILE:HD12	1.87	0.57
2:H:2:DT:C2'	2:H:3:DT:OP2	2.49	0.57
2:E:2:DT:C2'	2:E:3:DT:OP2	2.49	0.56
1:B:46:ASN:H	1:B:46:ASN:ND2	2.02	0.56
1:A:310:GLU:O	1:A:314:GLN:HG3	2.04	0.56
1:A:79:VAL:HG11	1:A:108:PRO:HG2	1.87	0.56
1:B:793:PRO:HG3	1:B:1000:ARG:NH2	2.21	0.56
1:B:159:ILE:CD1	1:B:210:GLU:HG2	2.35	0.56
1:A:47:ARG:HG2	1:A:97:ILE:HG22	1.86	0.56
1:B:921:ILE:HG23	1:B:1016:LEU:HD22	1.87	0.56
2:H:8:DT:C2'	2:H:9:DT:C5'	2.84	0.56
2:E:8:DT:C2'	2:E:9:DT:H5''	2.35	0.56
1:B:983:PHE:O	1:B:985:ARG:N	2.37	0.56
1:A:760:CYS:SG	1:A:776:PRO:HB2	2.45	0.56
1:A:159:ILE:CD1	1:A:210:GLU:HG2	2.36	0.56
1:A:628:ASN:OD1	1:A:630:PRO:HD2	2.06	0.56
1:A:510:ALA:HB3	1:A:541:LYS:HE2	1.88	0.56
1:A:524:GLU:HB3	1:A:560:VAL:HB	1.86	0.56
1:A:714:THR:HG22	1:A:716:GLU:H	1.71	0.56
1:B:47:ARG:NH1	1:B:122:PRO:HB2	2.20	0.56
1:B:471:SER:O	1:B:474:GLU:HG2	2.06	0.56
2:E:14:DT:H3'	2:E:14:DT:H6	1.71	0.56
1:B:992:LEU:HD13	1:B:1024:ARG:HH11	1.71	0.55
1:A:101:GLU:CD	1:A:270:ARG:HH21	2.08	0.55
1:A:359:ARG:HD3	1:A:359:ARG:C	2.27	0.55
1:B:493:CYS:O	1:B:496:GLN:CG	2.54	0.55
1:A:935:PRO:HB2	1:A:962:MET:HB2	1.89	0.55
1:A:471:SER:O	1:A:474:GLU:HG2	2.06	0.55
2:H:14:DT:H3'	2:H:14:DT:H6	1.71	0.55
1:B:840:LYS:HD2	1:B:1034:HIS:HD2	1.72	0.55
1:A:874:TYR:CE2	1:A:1054:HIS:HB3	2.42	0.55
1:B:524:GLU:HB3	1:B:560:VAL:HB	1.89	0.54
1:A:459:ARG:HG2	1:A:459:ARG:NH1	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:HH21	1:B:110:ILE:HG21	1.71	0.54
2:E:8:DT:C2'	2:E:9:DT:C5'	2.85	0.54
1:A:948:LEU:HD11	1:A:967:THR:HG23	1.89	0.54
1:B:969:ASP:OD1	1:B:969:ASP:N	2.41	0.54
1:B:831:ASN:O	1:B:833:LYS:N	2.40	0.54
1:B:2:GLU:O	1:B:3:PRO:O	2.26	0.54
1:B:242:PRO:HG2	1:B:330:GLU:OE2	2.08	0.54
1:A:714:THR:O	1:A:718:ILE:HG12	2.08	0.53
1:B:924:LEU:O	1:B:928:PHE:HD2	1.90	0.53
1:B:745:MET:CB	2:H:8:DT:H5'	2.39	0.53
1:B:101:GLU:CD	1:B:270:ARG:HH21	2.12	0.53
1:A:372:ARG:O	1:A:373:ALA:HB3	2.09	0.53
1:B:593:ARG:HG2	1:B:597:ILE:HD12	1.90	0.53
1:B:214:TYR:CE2	1:B:338:LYS:HA	2.43	0.53
1:A:533:LYS:HZ1	2:E:11:DT:H5'	1.71	0.53
1:B:459:ARG:NH1	1:B:459:ARG:HG2	2.18	0.53
1:A:503:ARG:HD2	1:A:508:MET:HG3	1.89	0.53
1:A:481:GLY:HA2	1:A:483:LEU:HG	1.89	0.53
1:A:831:ASN:O	1:A:833:LYS:N	2.42	0.53
1:A:978:LEU:HD21	1:A:980:LEU:HD21	1.89	0.53
1:B:533:LYS:HZ3	2:H:11:DT:H5'	1.72	0.53
1:A:493:CYS:O	1:A:496:GLN:CG	2.56	0.53
1:B:174:SER:HB3	1:B:179:ARG:HD2	1.91	0.53
2:E:14:DT:C6	2:E:14:DT:H3'	2.44	0.53
1:A:910:GLY:HA2	2:E:3:DT:C7	2.29	0.53
1:B:503:ARG:HD2	1:B:508:MET:HG3	1.91	0.53
1:A:104:CYS:O	1:A:105:THR:CB	2.56	0.52
1:A:678:TYR:HB2	1:A:768:ILE:HG12	1.89	0.52
1:B:298:LEU:HD11	1:B:335:LEU:HB2	1.92	0.52
1:B:260:LEU:CD1	1:B:295:VAL:HG22	2.39	0.52
1:A:84:ARG:HH21	1:A:110:ILE:HG21	1.75	0.52
1:B:58:ASN:O	1:B:62:ALA:HB3	2.09	0.52
1:A:897:ASN:HB3	1:A:1043:ASP:HA	1.90	0.52
1:A:945:ARG:NH1	2:E:5:DT:OP1	2.43	0.52
1:A:274:LYS:HE3	2:E:12:DT:OP2	2.08	0.52
2:H:14:DT:H3'	2:H:14:DT:C6	2.44	0.52
1:A:480:VAL:HG21	1:A:513:LEU:CD1	2.39	0.52
1:A:507:PRO:O	1:A:508:MET:CB	2.57	0.52
1:B:481:GLY:HA2	1:B:483:LEU:HG	1.90	0.52
1:B:859:LEU:HD12	1:B:1012:LYS:HD2	1.90	0.52
1:A:38:THR:HG21	1:A:97:ILE:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:948:LEU:HD11	1:B:967:THR:HG23	1.92	0.52
1:B:678:TYR:HB2	1:B:768:ILE:HG12	1.92	0.52
1:A:839:ASN:ND2	1:A:847:LEU:HB2	2.25	0.52
1:A:214:TYR:CE2	1:A:338:LYS:HA	2.45	0.52
1:A:745:MET:CB	2:E:8:DT:H5'	2.39	0.52
1:B:839:ASN:OD1	1:B:845:GLY:CA	2.58	0.52
1:B:311:HIS:HB3	1:B:334:LEU:HD11	1.91	0.52
1:A:40:LEU:HB3	1:A:71:ALA:O	2.10	0.52
1:B:480:VAL:HG21	1:B:513:LEU:CD1	2.40	0.51
1:B:678:TYR:OH	2:H:6:DT:O2	2.16	0.51
1:B:166:VAL:HG13	1:B:183:LEU:HB3	1.92	0.51
1:B:969:ASP:C	1:B:971:TYR:H	2.13	0.51
1:B:154:THR:HG23	1:B:157:MET:H	1.74	0.51
1:B:935:PRO:HB2	1:B:962:MET:HB2	1.92	0.51
1:A:2:GLU:CB	1:A:3:PRO:CD	2.89	0.51
1:A:492:VAL:O	1:A:493:CYS:HB2	2.10	0.51
1:B:528:LEU:O	1:B:531:LEU:CD1	2.59	0.51
1:B:104:CYS:O	1:B:105:THR:CB	2.59	0.51
1:B:433:HIS:ND1	1:B:585:SER:HB3	2.26	0.51
1:A:301:LYS:NZ	1:A:311:HIS:HD2	2.09	0.51
1:B:387:ILE:HG23	3:B:1101:SF4:S3	2.51	0.51
2:E:11:DT:H1'	2:E:12:DT:H71	1.93	0.51
1:B:325:ARG:HH22	1:B:531:LEU:H	1.59	0.51
1:B:47:ARG:HG2	1:B:97:ILE:HG22	1.92	0.51
1:A:839:ASN:OD1	1:A:845:GLY:CA	2.59	0.51
1:A:906:GLN:OE1	1:A:915:VAL:HG23	2.10	0.51
1:B:416:ASP:O	1:B:417:ALA:HB3	2.11	0.51
1:B:2:GLU:CB	1:B:3:PRO:HD3	2.37	0.51
1:A:171:ILE:HG12	1:A:259:SER:HB3	1.93	0.51
1:B:159:ILE:HD12	1:B:210:GLU:HG2	1.93	0.51
1:A:1048:GLU:HA	1:A:1048:GLU:OE1	2.09	0.51
1:B:301:LYS:HD3	2:H:15:DT:OP2	2.11	0.51
1:A:574:THR:HB	1:A:575:PRO:HD3	1.93	0.51
1:A:311:HIS:HB3	1:A:334:LEU:HD11	1.93	0.51
1:B:605:ILE:O	1:B:640:LEU:HD13	2.11	0.51
1:B:2:GLU:CB	1:B:3:PRO:CD	2.89	0.50
1:A:480:VAL:HG23	1:A:513:LEU:HD22	1.93	0.50
1:A:433:HIS:ND1	1:A:585:SER:HB3	2.26	0.50
1:B:462:HIS:O	1:B:466:TRP:CD1	2.65	0.50
1:B:507:PRO:O	1:B:508:MET:CB	2.59	0.50
1:A:582:LEU:HD22	1:A:774:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:GLU:O	1:A:567:GLU:HB2	2.12	0.50
1:A:159:ILE:HD12	1:A:210:GLU:HG2	1.93	0.50
1:B:150:SER:C	1:B:152:PRO:HD3	2.32	0.50
1:A:416:ASP:O	1:A:417:ALA:HB3	2.11	0.50
1:B:42:ARG:HB3	1:B:105:THR:CG2	2.41	0.50
1:B:480:VAL:HG23	1:B:513:LEU:HD22	1.93	0.50
1:A:528:LEU:O	1:A:531:LEU:CD1	2.59	0.50
1:A:790:GLN:O	1:A:1000:ARG:HG3	2.11	0.50
1:B:874:TYR:CE2	1:B:1054:HIS:HB3	2.46	0.50
1:B:677:SER:HB3	1:B:763:ASP:HB3	1.94	0.50
1:B:42:ARG:HB3	1:B:105:THR:HG21	1.94	0.50
2:H:1:DT:H1'	2:H:2:DT:C2	2.46	0.50
1:A:924:LEU:O	1:A:928:PHE:HD2	1.94	0.50
1:A:935:PRO:HA	1:A:938:ILE:HD12	1.92	0.50
1:A:47:ARG:HG2	1:A:97:ILE:CG2	2.42	0.50
1:B:38:THR:HG21	1:B:97:ILE:HG21	1.94	0.50
2:E:1:DT:H1'	2:E:2:DT:C2	2.47	0.50
1:B:918:ALA:O	1:B:922:VAL:HG23	2.11	0.50
1:B:880:SER:O	1:B:881:PRO:C	2.49	0.50
1:B:99:HIS:HB3	1:B:122:PRO:HG3	1.93	0.50
1:B:765:ALA:CB	1:B:785:LEU:HB3	2.42	0.50
1:B:453:SER:O	1:B:458:ASN:ND2	2.45	0.50
1:B:508:MET:HE2	1:B:508:MET:HA	1.94	0.50
1:A:445:TRP:CB	1:A:579:LEU:HD11	2.42	0.49
1:B:891:ASN:O	1:B:1012:LYS:NZ	2.39	0.49
1:B:310:GLU:O	1:B:314:GLN:HG3	2.11	0.49
2:H:11:DT:H1'	2:H:12:DT:H71	1.93	0.49
1:B:935:PRO:HA	1:B:938:ILE:HD12	1.94	0.49
1:B:906:GLN:OE1	1:B:915:VAL:HG23	2.12	0.49
1:B:832:ARG:NH1	1:B:856:ASN:OD1	2.44	0.49
1:B:760:CYS:SG	1:B:776:PRO:HB2	2.52	0.49
1:A:462:HIS:O	1:A:466:TRP:CD1	2.65	0.49
1:A:452:GLU:OE2	1:A:452:GLU:HA	2.13	0.49
1:B:359:ARG:C	1:B:359:ARG:HD3	2.33	0.49
1:A:465:ILE:HG23	1:A:564:ASP:OD2	2.13	0.49
1:A:503:ARG:CD	1:A:508:MET:HG3	2.43	0.49
1:B:471:SER:HA	1:B:474:GLU:OE2	2.13	0.49
1:A:138:LEU:O	1:A:142:VAL:HG23	2.12	0.49
1:A:2:GLU:CB	1:A:3:PRO:HD3	2.37	0.49
1:B:2:GLU:O	1:B:3:PRO:C	2.51	0.49
1:A:880:SER:O	1:A:881:PRO:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ASN:HB3	1:A:565:ARG:CG	2.43	0.49
1:B:910:GLY:HA2	2:H:3:DT:H71	1.93	0.49
1:B:521:LEU:O	1:B:530:ALA:O	2.31	0.49
1:A:150:SER:C	1:A:152:PRO:HD3	2.33	0.49
1:B:492:VAL:O	1:B:493:CYS:HB2	2.13	0.49
1:B:929:ILE:CD1	1:B:960:VAL:HG11	2.43	0.49
1:A:197:MET:HB3	1:A:727:LEU:HD22	1.95	0.49
1:B:1020:SER:O	1:B:1023:LYS:HG2	2.13	0.49
1:B:638:VAL:HG11	1:B:662:LEU:HD11	1.94	0.48
1:A:529:PHE:O	1:A:530:ALA:HB3	2.12	0.48
1:A:969:ASP:C	1:A:971:TYR:H	2.17	0.48
1:A:591:ARG:NH1	1:A:781:ARG:O	2.46	0.48
1:A:2:GLU:O	1:A:3:PRO:O	2.32	0.48
1:B:943:PRO:HD2	1:B:982:SER:O	2.13	0.48
1:B:659:ILE:HG21	1:B:686:ILE:HD13	1.95	0.48
1:B:275:GLY:CA	1:B:321:LEU:HD21	2.39	0.48
1:B:512:ASN:C	1:B:513:LEU:HD23	2.34	0.48
1:A:929:ILE:CD1	1:A:960:VAL:HG11	2.43	0.48
1:A:832:ARG:NH1	1:A:856:ASN:OD1	2.47	0.48
1:B:880:SER:N	1:B:881:PRO:CD	2.76	0.48
1:A:154:THR:HG23	1:A:157:MET:H	1.79	0.48
1:A:969:ASP:N	1:A:969:ASP:OD1	2.47	0.48
1:A:136:ARG:HD2	1:A:393:THR:HG21	1.95	0.48
1:A:453:SER:HB2	1:A:572:ILE:CG2	2.43	0.48
1:B:591:ARG:NH1	1:B:781:ARG:O	2.47	0.48
1:B:503:ARG:CD	1:B:508:MET:HG3	2.44	0.47
1:A:47:ARG:NH1	1:A:123:ASP:OD1	2.47	0.47
1:B:84:ARG:HB2	1:B:112:ASP:HB3	1.96	0.47
1:B:83:LEU:HD23	1:B:87:TRP:O	2.14	0.47
1:B:102:GLY:HA3	1:B:116:GLY:HA2	1.96	0.47
1:B:703:SER:HB3	1:B:714:THR:HG21	1.96	0.47
2:E:12:DT:H2"	2:E:13:DT:OP2	2.14	0.47
1:B:574:THR:HB	1:B:575:PRO:HD3	1.97	0.47
1:B:102:GLY:CA	1:B:116:GLY:HA2	2.44	0.47
1:A:350:LEU:O	1:A:354:GLU:HB2	2.14	0.47
1:A:879:ASP:C	1:A:881:PRO:HD2	2.35	0.47
1:B:491:ARG:O	1:B:493:CYS:N	2.46	0.47
1:A:918:ALA:O	1:A:922:VAL:HG23	2.15	0.47
1:B:372:ARG:O	1:B:373:ALA:HB3	2.14	0.47
1:A:455:SER:OG	1:A:798:ASN:HB2	2.14	0.47
1:A:526:ARG:HH11	1:A:526:ARG:CG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:SER:OG	1:A:498:LEU:HB3	2.15	0.47
1:A:673:VAL:HG13	1:A:739:ILE:HG12	1.97	0.47
1:A:333:TRP:CZ3	1:A:344:PRO:HB3	2.49	0.47
1:A:770:GLN:HG3	1:A:810:LEU:HB2	1.97	0.47
1:B:518:ARG:HD3	1:B:518:ARG:HA	1.73	0.47
1:B:2:GLU:H	1:B:6:GLU:HG3	1.80	0.47
1:A:512:ASN:C	1:A:513:LEU:HD23	2.34	0.47
1:A:301:LYS:O	1:A:336:TYR:HA	2.15	0.47
1:B:387:ILE:HG21	1:B:423:MET:HG2	1.97	0.47
1:B:215:LEU:O	1:B:218:PHE:HB2	2.15	0.47
1:A:985:ARG:HH12	1:A:993:GLY:H	1.63	0.47
1:B:240:SER:HA	1:B:248:ARG:HB2	1.97	0.47
1:B:533:LYS:HZ1	2:H:11:DT:H5'	1.80	0.47
1:A:880:SER:N	1:A:881:PRO:CD	2.75	0.47
1:B:480:VAL:CG2	1:B:513:LEU:HD22	2.45	0.47
1:B:452:GLU:OE2	1:B:452:GLU:HA	2.15	0.47
1:A:274:LYS:CE	2:E:12:DT:OP2	2.63	0.46
1:B:333:TRP:CZ3	1:B:344:PRO:HB3	2.49	0.46
1:B:862:PRO:HD2	1:B:932:GLY:HA3	1.97	0.46
2:H:12:DT:H2''	2:H:13:DT:OP2	2.15	0.46
1:B:998:ASP:OD1	1:B:1001:ARG:HG3	2.16	0.46
1:B:154:THR:HG22	1:B:157:MET:HG3	1.97	0.46
1:B:978:LEU:HD21	1:B:980:LEU:HD21	1.96	0.46
1:A:275:GLY:CA	1:A:321:LEU:HD21	2.42	0.46
1:B:301:LYS:O	1:B:336:TYR:HA	2.15	0.46
1:A:833:LYS:HD2	1:A:892:PRO:HD2	1.97	0.46
1:B:521:LEU:CD1	1:B:561:PHE:HB3	2.46	0.46
1:B:818:GLU:HA	1:B:821:VAL:HG23	1.98	0.46
1:B:40:LEU:HB3	1:B:71:ALA:O	2.15	0.46
1:A:387:ILE:HG21	1:A:423:MET:HG2	1.98	0.46
1:A:508:MET:HE2	1:A:508:MET:HA	1.98	0.46
1:A:524:GLU:N	1:A:560:VAL:O	2.48	0.46
1:B:47:ARG:NH1	1:B:123:ASP:OD1	2.48	0.46
1:B:192:ARG:NH2	1:B:193:HIS:CE1	2.83	0.46
1:A:679:THR:HG22	2:E:6:DT:O3'	2.16	0.46
1:B:566:GLU:O	1:B:567:GLU:CB	2.64	0.46
1:A:174:SER:HB3	1:A:179:ARG:HD2	1.97	0.46
1:A:183:LEU:O	1:A:187:THR:HG23	2.15	0.46
1:B:737:HIS:HA	1:B:738:PRO:HD3	1.86	0.46
1:A:765:ALA:CB	1:A:785:LEU:HB3	2.46	0.46
1:A:42:ARG:HB3	1:A:105:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:SER:OG	1:B:498:LEU:HB3	2.15	0.46
1:A:862:PRO:HD2	1:A:932:GLY:HA3	1.98	0.46
2:H:6:DT:H2"	2:H:7:DT:C6	2.51	0.46
1:A:521:LEU:HD11	1:A:561:PHE:HB3	1.96	0.46
1:A:491:ARG:O	1:A:493:CYS:N	2.47	0.46
1:A:888:GLU:OE1	1:A:888:GLU:HA	2.16	0.46
2:E:6:DT:H2"	2:E:7:DT:C6	2.51	0.46
1:A:670:GLY:HA2	1:B:729:HIS:NE2	2.31	0.46
1:A:929:ILE:HA	1:A:933:CYS:O	2.17	0.45
1:B:882:TRP:CZ3	1:B:883:LEU:HG	2.50	0.45
1:B:984:VAL:HG23	1:B:984:VAL:O	2.15	0.45
1:B:169:LYS:HZ2	1:B:187:THR:HG22	1.82	0.45
1:B:622:ASN:HA	1:B:625:LYS:HE2	1.97	0.45
1:A:83:LEU:HD23	1:A:87:TRP:O	2.17	0.45
1:A:101:GLU:OE1	1:A:270:ARG:NH2	2.49	0.45
1:B:99:HIS:HB2	1:B:122:PRO:HG2	1.98	0.45
1:A:42:ARG:HB3	1:A:105:THR:HG21	1.99	0.45
1:A:102:GLY:CA	1:A:116:GLY:HA2	2.46	0.45
1:B:1046:SER:O	1:B:1052:LEU:HD12	2.17	0.45
1:A:737:HIS:HA	1:A:738:PRO:HD3	1.88	0.45
1:A:489:VAL:CG1	1:A:497:TYR:HB3	2.47	0.45
1:B:1048:GLU:OE1	1:B:1048:GLU:HA	2.16	0.45
1:A:167:PHE:C	1:A:167:PHE:CD2	2.89	0.45
1:B:136:ARG:HD2	1:B:393:THR:HG21	1.97	0.45
1:A:495:GLY:O	1:A:549:ASP:CA	2.32	0.45
1:B:489:VAL:CG1	1:B:497:TYR:HB3	2.47	0.45
1:A:518:ARG:HA	1:A:518:ARG:HD3	1.63	0.45
1:A:895:PHE:CD2	1:A:1015:LEU:HB2	2.51	0.45
1:B:529:PHE:O	1:B:530:ALA:HB3	2.16	0.45
2:E:9:DT:O3'	2:E:10:DT:O4'	2.34	0.45
1:A:521:LEU:CD1	1:A:561:PHE:HB3	2.47	0.45
1:A:521:LEU:O	1:A:530:ALA:O	2.34	0.45
1:A:250:SER:OG	1:A:287:ARG:NH2	2.50	0.45
1:A:950:ILE:O	1:A:954:LEU:HG	2.17	0.45
1:B:521:LEU:HD11	1:B:561:PHE:HB3	1.98	0.45
1:B:240:SER:HA	1:B:248:ARG:CB	2.47	0.45
1:B:550:ARG:HH11	1:B:550:ARG:HB3	1.82	0.45
1:A:992:LEU:HD13	1:A:1024:ARG:NH1	2.31	0.45
1:A:969:ASP:OD1	1:A:1001:ARG:NH2	2.50	0.45
1:B:301:LYS:NZ	1:B:311:HIS:HD2	2.15	0.44
1:B:596:ILE:O	1:B:813:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:HB3	1:A:531:LEU:HD11	1.99	0.44
1:A:559:THR:HB	1:A:561:PHE:CZ	2.52	0.44
1:B:505:ASN:CG	1:B:506:GLY:N	2.71	0.44
1:A:998:ASP:OD2	1:A:1000:ARG:NH1	2.50	0.44
1:B:524:GLU:N	1:B:560:VAL:O	2.50	0.44
1:B:416:ASP:O	1:B:417:ALA:CB	2.65	0.44
1:B:508:MET:CE	1:B:508:MET:HA	2.47	0.44
1:A:483:LEU:O	1:A:560:VAL:HA	2.18	0.44
1:B:559:THR:HB	1:B:561:PHE:CZ	2.52	0.44
1:B:518:ARG:O	1:B:565:ARG:HA	2.17	0.44
1:A:568:ARG:O	1:A:569:HIS:HB3	2.17	0.44
1:B:154:THR:HG22	1:B:157:MET:CG	2.47	0.44
1:A:937:ASP:HB3	1:A:977:SER:HB2	2.00	0.44
1:A:224:ASP:O	1:A:235:PRO:HD3	2.17	0.44
1:A:943:PRO:HD2	1:A:982:SER:O	2.18	0.44
2:H:9:DT:O3'	2:H:10:DT:O4'	2.35	0.44
1:A:102:GLY:HA3	1:A:116:GLY:HA2	1.99	0.44
1:A:480:VAL:CG2	1:A:513:LEU:HD22	2.47	0.44
1:B:868:ARG:HH21	1:B:884:ALA:HA	1.82	0.44
2:H:14:DT:C6	2:H:14:DT:C3'	3.01	0.44
1:A:2:GLU:O	1:A:3:PRO:C	2.55	0.44
1:B:459:ARG:HH11	1:B:459:ARG:CA	2.30	0.44
1:A:325:ARG:HH22	1:A:531:LEU:H	1.64	0.44
1:B:473:LEU:HB2	1:B:479:CYS:HB3	2.00	0.44
1:B:582:LEU:HD22	1:B:774:LEU:HD21	2.00	0.44
1:B:495:GLY:O	1:B:549:ASP:CA	2.30	0.44
1:A:494:ASP:CG	1:A:495:GLY:N	2.71	0.44
1:B:998:ASP:OD2	1:B:1000:ARG:NH1	2.50	0.44
1:A:508:MET:CE	1:A:508:MET:HA	2.48	0.44
1:B:714:THR:O	1:B:718:ILE:HG12	2.18	0.44
1:A:121:TYR:N	1:A:122:PRO:HD3	2.32	0.44
1:A:604:PHE:CZ	1:A:820:ALA:HA	2.53	0.44
1:B:879:ASP:C	1:B:881:PRO:HD2	2.37	0.44
1:B:929:ILE:HA	1:B:933:CYS:O	2.18	0.44
1:B:416:ASP:HB3	1:B:417:ALA:H	1.67	0.44
1:B:604:PHE:CZ	1:B:820:ALA:HA	2.52	0.44
2:E:14:DT:C6	2:E:14:DT:C3'	3.01	0.43
1:B:568:ARG:O	1:B:569:HIS:HB3	2.18	0.43
2:H:2:DT:N1	2:H:3:DT:H72	2.32	0.43
1:A:872:GLN:OE1	1:A:877:TYR:HD1	2.01	0.43
1:B:457:ASP:O	1:B:460:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:NE	1:A:403:CYS:SG	2.75	0.43
1:A:84:ARG:HB2	1:A:112:ASP:HB3	2.00	0.43
1:A:416:ASP:O	1:A:417:ALA:CB	2.66	0.43
1:A:729:HIS:NE2	1:B:670:GLY:HA2	2.32	0.43
1:A:650:MET:O	1:A:653:THR:HG23	2.18	0.43
1:A:473:LEU:HB2	1:A:479:CYS:HB3	2.01	0.43
1:B:828:TYR:CD1	1:B:828:TYR:N	2.86	0.43
2:H:11:DT:H1'	2:H:12:DT:C7	2.49	0.43
1:A:335:LEU:O	1:A:341:GLN:O	2.37	0.43
1:A:301:LYS:HD3	2:E:15:DT:OP2	2.18	0.43
1:B:634:ALA:HA	1:B:822:VAL:HG11	2.01	0.43
2:E:12:DT:H72	2:E:13:DT:O4	2.19	0.43
1:B:612:LEU:N	1:B:612:LEU:HD12	2.33	0.43
1:A:550:ARG:HH11	1:A:550:ARG:HB3	1.84	0.43
1:A:707:HIS:HA	1:A:708:PRO:HD3	1.92	0.43
1:A:622:ASN:HA	1:A:625:LYS:HE2	2.01	0.43
1:B:572:ILE:C	1:B:575:PRO:HD2	2.39	0.43
1:A:453:SER:O	1:A:458:ASN:ND2	2.51	0.43
1:A:273:LEU:HD21	1:A:359:ARG:HG3	2.00	0.43
1:B:171:ILE:HG12	1:B:259:SER:HB3	2.01	0.43
1:A:1046:SER:O	1:A:1052:LEU:HD12	2.18	0.43
1:B:269:PRO:HD2	1:B:526:ARG:HH22	1.84	0.43
1:B:99:HIS:HB3	1:B:122:PRO:CG	2.49	0.43
1:A:992:LEU:HD13	1:A:1024:ARG:HH11	1.83	0.43
1:A:202:LEU:HD13	1:A:207:ILE:HD11	2.01	0.43
1:B:657:THR:HG23	1:B:689:LYS:HZ2	1.83	0.42
1:B:528:LEU:HB3	1:B:531:LEU:HD11	2.01	0.42
1:B:474:GLU:HB3	1:B:479:CYS:O	2.19	0.42
1:B:653:THR:OG1	1:B:824:LEU:HB3	2.18	0.42
1:B:242:PRO:HD2	1:B:330:GLU:HB3	2.01	0.42
1:B:882:TRP:CE3	1:B:883:LEU:HG	2.54	0.42
1:B:532:SER:HB2	1:B:550:ARG:HB2	2.02	0.42
1:A:157:MET:HA	2:E:14:DT:H2'	2.00	0.42
1:A:462:HIS:HD2	1:A:465:ILE:CD1	2.33	0.42
1:B:250:SER:OG	1:B:287:ARG:NH2	2.51	0.42
1:B:155:ARG:O	1:B:159:ILE:HG12	2.19	0.42
1:A:703:SER:HB3	1:A:714:THR:HG21	2.00	0.42
1:B:924:LEU:O	1:B:928:PHE:CD2	2.71	0.42
1:B:183:LEU:O	1:B:187:THR:CG2	2.66	0.42
1:B:236:GLN:HA	1:B:252:CYS:O	2.19	0.42
1:B:167:PHE:C	1:B:167:PHE:CD2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LYS:HD2	2:H:12:DT:OP2	2.19	0.42
1:A:471:SER:HA	1:A:474:GLU:OE2	2.19	0.42
1:A:839:ASN:OD1	1:A:845:GLY:HA2	2.20	0.42
1:A:1020:SER:O	1:A:1023:LYS:HG2	2.19	0.42
1:B:459:ARG:NH1	1:B:459:ARG:CG	2.76	0.42
1:B:839:ASN:OD1	1:B:845:GLY:HA2	2.19	0.42
1:A:700:LEU:HD22	1:A:749:HIS:NE2	2.35	0.42
1:B:459:ARG:NH1	1:B:459:ARG:HA	2.33	0.42
1:B:937:ASP:HB3	1:B:977:SER:HB2	2.01	0.42
2:H:1:DT:H2'	2:H:2:DT:O4'	2.20	0.42
1:A:2:GLU:H	1:A:6:GLU:HG3	1.85	0.42
1:A:530:ALA:O	1:A:531:LEU:HB2	2.20	0.42
1:B:166:VAL:HG22	1:B:187:THR:HG21	2.02	0.42
1:B:40:LEU:HD21	1:B:49:LEU:HB2	2.02	0.42
1:B:770:GLN:HG3	1:B:810:LEU:HB2	2.02	0.42
1:B:197:MET:HB3	1:B:727:LEU:HD22	2.02	0.42
1:B:455:SER:OG	1:B:798:ASN:HB2	2.19	0.42
1:A:579:LEU:HD23	1:A:579:LEU:HA	1.78	0.42
1:B:485:ARG:NH1	1:B:487:GLU:O	2.52	0.42
1:A:240:SER:HA	1:A:248:ARG:HB2	2.02	0.42
1:A:505:ASN:CG	1:A:506:GLY:N	2.74	0.41
1:B:483:LEU:O	1:B:560:VAL:HA	2.20	0.41
1:B:66:ARG:HH22	1:B:80:LEU:HD11	1.85	0.41
2:E:8:DT:H71	2:E:9:DT:H73	2.02	0.41
1:A:320:LEU:O	1:A:321:LEU:C	2.58	0.41
1:B:323:GLN:C	1:B:325:ARG:H	2.23	0.41
1:B:985:ARG:HH12	1:B:993:GLY:H	1.65	0.41
1:A:928:PHE:O	1:A:933:CYS:HB3	2.20	0.41
1:A:569:HIS:CG	1:A:570:GLY:N	2.88	0.41
1:B:165:GLU:HG2	1:B:169:LYS:HE3	2.02	0.41
1:B:47:ARG:HG2	1:B:97:ILE:CG2	2.50	0.41
1:B:929:ILE:HG23	1:B:935:PRO:HD3	2.02	0.41
1:A:44:VAL:HG23	1:A:45:ASP:N	2.34	0.41
1:A:274:LYS:HD2	2:E:12:DT:OP2	2.20	0.41
1:B:484:VAL:HG21	1:B:504:LYS:HE2	2.02	0.41
1:A:126:ILE:O	1:A:273:LEU:HA	2.20	0.41
1:B:441:TYR:CG	1:B:597:ILE:HG12	2.55	0.41
1:B:214:TYR:CD2	1:B:338:LYS:HA	2.55	0.41
1:A:301:LYS:HZ3	1:A:311:HIS:HD2	1.68	0.41
1:A:518:ARG:CD	2:E:9:DT:H72	2.50	0.41
1:A:657:THR:OG1	4:A:1102:ADP:O2A	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ASP:OD2	1:A:565:ARG:NH2	2.53	0.41
1:A:243:SER:O	1:A:248:ARG:CG	2.69	0.41
1:B:571:ASP:O	1:B:573:SER:N	2.54	0.41
1:A:312:ARG:CZ	1:A:345:VAL:HG22	2.50	0.41
1:B:517:ASP:O	1:B:535:TYR:HB2	2.21	0.41
2:E:11:DT:H1'	2:E:12:DT:C7	2.49	0.41
1:A:40:LEU:HA	1:A:47:ARG:O	2.21	0.41
1:A:372:ARG:O	1:A:373:ALA:CB	2.68	0.41
1:B:497:TYR:HB2	1:B:499:HIS:HE1	1.85	0.41
2:E:1:DT:H2'	2:E:2:DT:O4'	2.20	0.41
1:A:459:ARG:NH1	1:A:459:ARG:HA	2.35	0.41
1:B:895:PHE:CD2	1:B:1015:LEU:HB2	2.56	0.41
2:E:8:DT:C7	2:E:9:DT:H71	2.51	0.41
1:A:512:ASN:O	1:A:565:ARG:NH1	2.54	0.41
1:A:929:ILE:HG23	1:A:935:PRO:HD3	2.02	0.41
1:A:214:TYR:CD2	1:A:338:LYS:HA	2.56	0.41
1:B:903:ALA:N	1:B:904:PRO:HD3	2.36	0.41
1:B:65:LYS:HD3	1:B:67:LEU:HD21	2.03	0.41
1:B:21:VAL:N	1:B:22:PRO:HD2	2.35	0.41
1:A:760:CYS:HB2	1:A:780:SER:CB	2.51	0.41
1:B:101:GLU:OE1	1:B:270:ARG:NH2	2.53	0.40
1:A:917:GLU:O	1:A:921:ILE:HG12	2.20	0.40
1:A:566:GLU:O	1:A:567:GLU:CB	2.69	0.40
1:A:791:GLN:O	1:A:1000:ARG:HG2	2.21	0.40
1:A:315:VAL:O	1:A:318:TYR:HB2	2.21	0.40
1:B:275:GLY:HA3	1:B:321:LEU:CD2	2.42	0.40
1:B:325:ARG:NH2	1:B:531:LEU:H	2.18	0.40
1:A:226:MET:HG2	1:A:256:VAL:HB	2.04	0.40
1:A:911:GLY:C	1:A:946:GLN:HE21	2.24	0.40
1:A:494:ASP:CG	1:A:495:GLY:H	2.24	0.40
1:A:104:CYS:SG	1:A:107:GLU:O	2.77	0.40
1:A:459:ARG:CA	1:A:459:ARG:HH11	2.34	0.40
1:A:971:TYR:O	1:A:972:GLN:C	2.59	0.40
1:A:240:SER:HA	1:A:248:ARG:CB	2.50	0.40
1:A:457:ASP:O	1:A:460:LYS:HE2	2.21	0.40
1:B:367:LEU:HD11	1:B:459:ARG:HH21	1.87	0.40
1:B:1047:ARG:HH21	1:B:1056:LEU:HD22	1.86	0.40
1:A:718:ILE:H	1:A:718:ILE:HG12	1.78	0.40
1:A:677:SER:HB3	1:A:763:ASP:HB3	2.03	0.40
2:H:12:DT:H72	2:H:13:DT:O4	2.21	0.40
1:A:46:ASN:N	1:A:46:ASN:ND2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ARG:HA	1:B:372:ARG:NE	2.37	0.40
1:B:243:SER:O	1:B:248:ARG:CG	2.69	0.40
1:B:519:ILE:HA	1:B:564:ASP:O	2.21	0.40
1:A:21:VAL:N	1:A:22:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1038/1056 (98%)	897 (86%)	109 (10%)	32 (3%)	5	25
1	B	1038/1056 (98%)	895 (86%)	111 (11%)	32 (3%)	5	25
All	All	2076/2112 (98%)	1792 (86%)	220 (11%)	64 (3%)	5	25

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	60	ARG
1	A	375	PRO
1	A	505	ASN
1	A	508	MET
1	A	557	ALA
1	A	567	GLU
1	A	832	ARG
1	A	984	VAL
1	B	2	GLU
1	B	60	ARG
1	B	375	PRO
1	B	505	ASN
1	B	508	MET

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Mol	Chain	Res	Type
1	B	557	ALA
1	B	567	GLU
1	B	569	HIS
1	B	832	ARG
1	B	984	VAL
1	A	105	THR
1	A	250	SER
1	A	417	ALA
1	A	493	CYS
1	A	530	ALA
1	A	566	GLU
1	A	569	HIS
1	A	988	GLU
1	B	105	THR
1	B	250	SER
1	B	324	GLU
1	B	417	ALA
1	B	493	CYS
1	B	530	ALA
1	B	988	GLU
1	B	1019	VAL
1	A	103	ASP
1	A	721	SER
1	A	874	TYR
1	A	1019	VAL
1	B	721	SER
1	B	874	TYR
1	A	3	PRO
1	A	40	LEU
1	A	108	PRO
1	A	324	GLU
1	A	881	PRO
1	B	3	PRO
1	B	40	LEU
1	B	103	ASP
1	B	108	PRO
1	B	228	LYS
1	B	881	PRO
1	A	228	LYS
1	A	420	PRO
1	B	420	PRO
1	B	970	LYS

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Mol	Chain	Res	Type
1	A	477	GLY
1	B	21	VAL
1	B	102	GLY
1	A	102	GLY
1	A	303	GLY
1	A	492	VAL
1	B	477	GLY
1	B	492	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	
1	A	930/936 (99%)	831 (89%)	99 (11%)	8	30
1	B	930/936 (99%)	830 (89%)	100 (11%)	8	29
All	All	1860/1872 (99%)	1661 (89%)	199 (11%)	8	30

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	25	GLU
1	A	46	ASN
1	A	47	ARG
1	A	54	GLU
1	A	66	ARG
1	A	70	THR
1	A	93	GLU
1	A	100	LEU
1	A	101	GLU
1	A	109	TRP
1	A	111	ILE
1	A	113	ASP
1	A	140	ARG
1	A	144	SER

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Mol	Chain	Res	Type
1	A	164	HIS
1	A	174	SER
1	A	178	GLU
1	A	183	LEU
1	A	185	LEU
1	A	187	THR
1	A	188	LEU
1	A	191	VAL
1	A	208	LEU
1	A	210	GLU
1	A	223	GLU
1	A	232	SER
1	A	240	SER
1	A	265	SER
1	A	279	VAL
1	A	280	THR
1	A	287	ARG
1	A	289	CYS
1	A	321	LEU
1	A	334	LEU
1	A	359	ARG
1	A	367	LEU
1	A	369	ARG
1	A	372	ARG
1	A	378	GLU
1	A	393	THR
1	A	400	ILE
1	A	410	VAL
1	A	411	GLU
1	A	416	ASP
1	A	424	LEU
1	A	458	ASN
1	A	459	ARG
1	A	482	ASN
1	A	485	ARG
1	A	491	ARG
1	A	502	GLN
1	A	505	ASN
1	A	513	LEU
1	A	518	ARG
1	A	526	ARG
1	A	531	LEU

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Mol	Chain	Res	Type
1	A	540	ASN
1	A	546	CYS
1	A	547	LEU
1	A	550	ARG
1	A	556	PRO
1	A	559	THR
1	A	568	ARG
1	A	586	THR
1	A	601	GLU
1	A	609	SER
1	A	615	ASP
1	A	632	ARG
1	A	673	VAL
1	A	683	VAL
1	A	723	SER
1	A	738	PRO
1	A	769	SER
1	A	780	SER
1	A	781	ARG
1	A	816	ARG
1	A	818	GLU
1	A	822	VAL
1	A	824	LEU
1	A	832	ARG
1	A	841	LEU
1	A	858	VAL
1	A	859	LEU
1	A	901	VAL
1	A	906	GLN
1	A	913	SER
1	A	916	THR
1	A	946	GLN
1	A	949	ARG
1	A	957	ARG
1	A	962	MET
1	A	968	VAL
1	A	969	ASP
1	A	984	VAL
1	A	985	ARG
1	A	987	ASN
1	A	1000	ARG
1	A	1047	ARG

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Mol	Chain	Res	Type
1	B	1	MET
1	B	25	GLU
1	B	46	ASN
1	B	47	ARG
1	B	54	GLU
1	B	66	ARG
1	B	70	THR
1	B	100	LEU
1	B	101	GLU
1	B	109	TRP
1	B	111	ILE
1	B	113	ASP
1	B	144	SER
1	B	164	HIS
1	B	174	SER
1	B	178	GLU
1	B	183	LEU
1	B	185	LEU
1	B	187	THR
1	B	188	LEU
1	B	191	VAL
1	B	208	LEU
1	B	210	GLU
1	B	223	GLU
1	B	233	GLU
1	B	240	SER
1	B	258	LYS
1	B	265	SER
1	B	279	VAL
1	B	280	THR
1	B	287	ARG
1	B	289	CYS
1	B	321	LEU
1	B	334	LEU
1	B	350	LEU
1	B	359	ARG
1	B	367	LEU
1	B	369	ARG
1	B	370	VAL
1	B	372	ARG
1	B	378	GLU
1	B	393	THR

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Mol	Chain	Res	Type
1	B	400	ILE
1	B	410	VAL
1	B	411	GLU
1	B	416	ASP
1	B	424	LEU
1	B	458	ASN
1	B	459	ARG
1	B	482	ASN
1	B	485	ARG
1	B	491	ARG
1	B	502	GLN
1	B	505	ASN
1	B	513	LEU
1	B	518	ARG
1	B	526	ARG
1	B	531	LEU
1	B	540	ASN
1	B	546	CYS
1	B	547	LEU
1	B	550	ARG
1	B	556	PRO
1	B	559	THR
1	B	562	ARG
1	B	565	ARG
1	B	586	THR
1	B	601	GLU
1	B	609	SER
1	B	615	ASP
1	B	632	ARG
1	B	657	THR
1	B	673	VAL
1	B	723	SER
1	B	769	SER
1	B	780	SER
1	B	781	ARG
1	B	816	ARG
1	B	818	GLU
1	B	822	VAL
1	B	824	LEU
1	B	832	ARG
1	B	841	LEU
1	B	858	VAL

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Mol	Chain	Res	Type
1	B	859	LEU
1	B	901	VAL
1	B	906	GLN
1	B	913	SER
1	B	916	THR
1	B	946	GLN
1	B	949	ARG
1	B	957	ARG
1	B	962	MET
1	B	968	VAL
1	B	969	ASP
1	B	984	VAL
1	B	985	ARG
1	B	987	ASN
1	B	1000	ARG
1	B	1047	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	77	HIS
1	A	311	HIS
1	A	462	HIS
1	A	704	HIS
1	A	817	ASN
1	A	946	GLN
1	B	77	HIS
1	B	458	ASN
1	B	462	HIS
1	B	817	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	SF4	A	1101	1	0,12,12	0.00	-	0,24,24	0.00	-
4	ADP	A	1102	-	24,29,29	0.97	1 (4%)	23,45,45	1.75	1 (4%)
3	SF4	B	1101	1	0,12,12	0.00	-	0,24,24	0.00	-
4	ADP	B	1102	-	24,29,29	1.07	1 (4%)	23,45,45	1.75	3 (13%)

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	SF4	A	1101	1	-	0/0/48/48	0/6/5/5
4	ADP	A	1102	-	-	0/12/32/32	0/3/3/3
3	SF4	B	1101	1	-	0/0/48/48	0/6/5/5
4	ADP	B	1102	-	-	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)
4	A	1102	ADP	C5-C4	3.06	1.47	1.40
4	B	1102	ADP	C5-C4	3.40	1.48	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	ADP	N3-C2-N1	-6.75	123.57	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1102	ADP	N3-C2-N1	-6.46	123.80	128.87
4	B	1102	ADP	C1'-N9-C4	-2.04	124.53	126.81
4	B	1102	ADP	C2-N1-C6	2.14	122.58	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1102	ADP	2	0
3	B	1101	SF4	1	0
4	B	1102	ADP	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1046/1056 (99%)	-0.26	26 (2%) 61 35	31, 62, 128, 168	0
1	B	1046/1056 (99%)	-0.16	36 (3%) 49 23	30, 67, 136, 165	0
2	E	17/17 (100%)	0.80	3 (17%) 2 1	72, 116, 169, 173	0
2	H	17/17 (100%)	0.67	3 (17%) 2 1	76, 120, 163, 171	0
All	All	2126/2146 (99%)	-0.19	68 (3%) 51 25	30, 65, 134, 173	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	478	ASN	8.5
1	B	457	ASP	6.5
1	A	507	PRO	4.6
1	B	245	GLY	4.1
1	A	505	ASN	4.0
1	B	877	TYR	3.9
1	A	21	VAL	3.8
2	E	1	DT	3.6
1	B	1050	GLU	3.6
1	B	415	ASP	3.5
1	A	478	ASN	3.5
1	B	395	LYS	3.4
1	A	457	ASP	3.3
2	E	17	DT	3.3
2	H	17	DT	3.3
1	B	20	ALA	3.2
1	A	244	ASP	3.0
1	A	395	LYS	2.9
1	A	569	HIS	2.8
1	A	471	SER	2.8
1	B	505	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	248	ARG	2.7
1	A	472	GLU	2.7
1	B	866	ASP	2.7
1	B	477	GLY	2.6
1	A	506	GLY	2.6
1	B	511	THR	2.6
1	B	506	GLY	2.6
1	B	878	SER	2.6
2	H	10	DT	2.5
1	A	375	PRO	2.5
1	A	20	ALA	2.5
1	B	248	ARG	2.5
2	H	1	DT	2.5
1	B	507	PRO	2.5
1	B	514	MET	2.5
2	E	10	DT	2.4
1	B	375	PRO	2.4
1	A	504	LYS	2.4
1	B	396	TYR	2.4
1	B	103	ASP	2.4
1	B	412	GLU	2.4
1	A	1050	GLU	2.4
1	B	471	SER	2.4
1	A	396	TYR	2.4
1	B	852	ASP	2.3
1	B	61	GLY	2.3
1	B	21	VAL	2.3
1	A	76	GLU	2.3
1	B	494	ASP	2.3
1	B	22	PRO	2.3
1	A	22	PRO	2.2
1	B	481	GLY	2.2
1	A	249	SER	2.2
1	B	244	ASP	2.2
1	B	517	ASP	2.2
1	B	63	GLU	2.2
1	B	473	LEU	2.1
1	A	245	GLY	2.1
1	A	953	ASP	2.1
1	B	504	LYS	2.1
1	B	488	PRO	2.1
1	A	415	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	59	GLU	2.0
1	B	567	GLU	2.0
1	B	1054	HIS	2.0
1	A	350	LEU	2.0
1	A	513	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ADP	B	1102	27/27	0.88	0.17	-0.46	69,77,107,108	0
4	ADP	A	1102	27/27	0.91	0.14	-1.31	63,74,100,101	0
3	SF4	A	1101	8/8	0.98	0.09	-1.63	67,69,70,76	0
3	SF4	B	1101	8/8	0.97	0.09	-1.71	69,72,74,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.