



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:57 AM GMT

PDB ID : 2JGD  
Title : E. COLI 2-OXOGLUTARATE DEHYDROGENASE (E1O)  
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Deposited on : 2007-02-12  
Resolution : 2.60 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

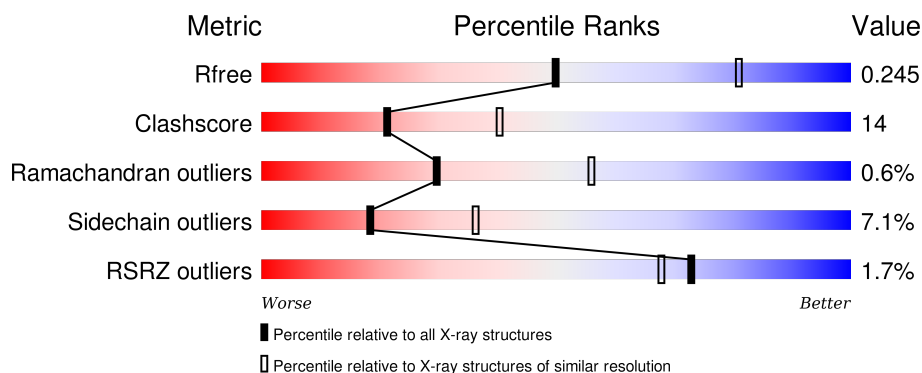
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	933	<div> <div>2%</div> <div>64%</div> <div>19%</div> <div>•</div> <div>13%</div> </div>
2	B	933	<div> <div>%</div> <div>66%</div> <div>17%</div> <div>•</div> <div>14%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13374 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 2-OXOGLUTARATE DEHYDROGENASE E1 COMPONENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	812	Total	C	N	O	S	0	2	0
			6323	4006	1118	1165	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	914	HIS	TYR	CONFLICT	UNP P0AFG3

- Molecule 2 is a protein called 2-OXOGLUTARATE DEHYDROGENASE E1 COMPONENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	807	Total	C	N	O	S	0	2	0
			6270	3968	1113	1156	33			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	579	ALA	GLY	CONFLICT	UNP P0AFG3

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

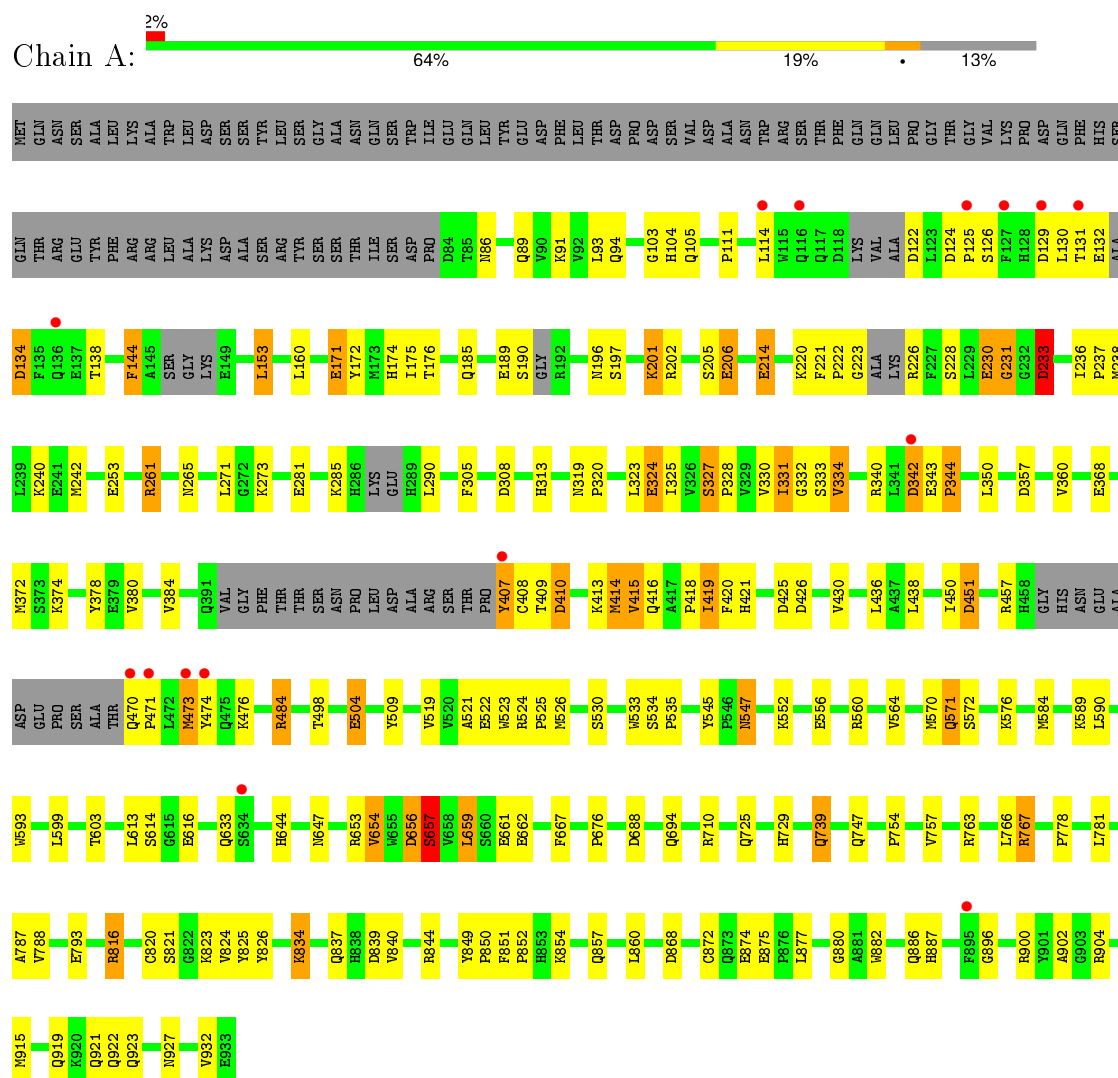
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	337	Total	O	0	0
			337	337		
4	B	398	Total	O	0	0
			398	398		

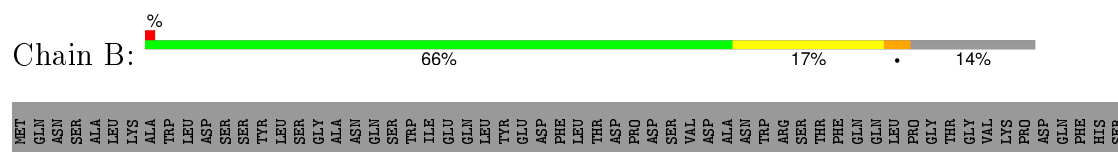
### 3 Residue-property plots

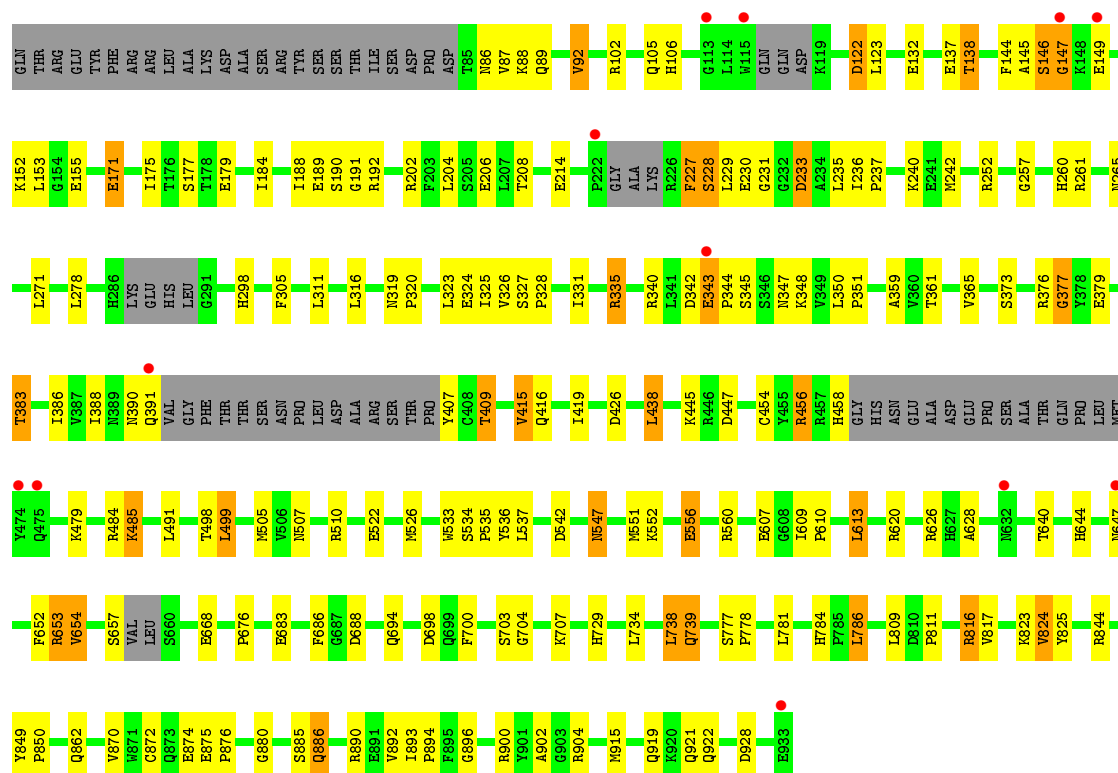
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 2-OXOGLUTARATE DEHYDROGENASE E1 COMPONENT



#### • Molecule 2: 2-OXOGLUTARATE DEHYDROGENASE E1 COMPONENT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.49 Å   142.49 Å   251.81 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.09 – 2.60 29.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.09-2.60) 99.9 (29.08-2.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.186   ,   0.250 0.183   ,   0.245	Depositor DCC
$R_{free}$ test set	4031 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 80382 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

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

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	0.55	0/6470	0.56	5/8761 (0.1%)
2	B	0.55	0/6415	0.56	4/8689 (0.0%)
All	All	0.55	0/12885	0.56	9/17450 (0.1%)

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	10
2	B	0	13
All	All	0	23

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	308	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	656	ASP	CB-CG-OD2	5.23	123.01	118.30
2	B	542	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	342	ASP	CB-CG-OD2	5.22	122.99	118.30
1	A	233	ASP	CB-CG-OD2	5.21	122.99	118.30
2	B	698	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	451	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	447	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	928	ASP	CB-CG-OD2	5.18	122.96	118.30

There are no chirality outliers.

All (23) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	144	PHE	Peptide
1	A	171	GLU	Peptide
1	A	226	ARG	Peptide
1	A	230	GLU	Peptide
1	A	231	GLY	Peptide
1	A	290	LEU	Peptide
1	A	342	ASP	Peptide
1	A	414	MET	Peptide
1	A	657	SER	Peptide
1	A	896	GLY	Peptide
2	B	144	PHE	Peptide
2	B	145	ALA	Peptide
2	B	146	SER	Peptide
2	B	147	GLY	Peptide
2	B	189	GLU	Peptide
2	B	190	SER	Peptide
2	B	191	GLY	Peptide
2	B	192	ARG	Peptide
2	B	227	PHE	Peptide
2	B	376	ARG	Peptide
2	B	377	GLY	Peptide
2	B	536	TYR	Peptide
2	B	896	GLY	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	6323	0	6069	201	0
2	B	6270	0	6013	159	0
3	A	23	0	12	0	0
3	B	23	0	12	0	0
4	A	337	0	0	15	0
4	B	398	0	0	17	0
All	All	13374	0	12106	352	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 14.

All (352) 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:A:767:ARG:HG2	1:A:767:ARG:O	1.37	1.13
2:B:343:GLU:HG2	2:B:343:GLU:O	1.36	1.13
2:B:824:VAL:HG22	2:B:874:GLU:HG3	1.26	1.10
2:B:560[B]:ARG:HH11	2:B:560[B]:ARG:HG3	1.11	1.07
1:A:242:MET:CE	1:A:384:VAL:HG11	1.87	1.04
1:A:228:SER:OG	1:A:230:GLU:HG3	1.62	0.98
1:A:242:MET:HE1	1:A:384:VAL:HG11	1.43	0.97
2:B:305:PHE:CZ	2:B:522:GLU:HG3	2.03	0.94
2:B:560[B]:ARG:HH11	2:B:560[B]:ARG:CG	1.81	0.94
2:B:343:GLU:CG	2:B:343:GLU:O	2.17	0.92
1:A:153:LEU:O	1:A:153:LEU:HD12	1.70	0.91
1:A:153:LEU:HD12	1:A:153:LEU:C	1.88	0.91
2:B:824:VAL:HG23	4:B:2313:HOH:O	1.72	0.90
2:B:335:ARG:NH2	2:B:377:GLY:CA	2.36	0.89
1:A:767:ARG:CG	1:A:767:ARG:O	2.19	0.87
1:A:904:ARG:NH2	1:A:921:GLN:HB2	1.89	0.87
2:B:825:TYR:CD2	2:B:844:ARG:HD2	2.10	0.86
1:A:236:ILE:HB	1:A:237:PRO:HD3	1.57	0.85
1:A:407:TYR:CD1	1:A:408:CYS:N	2.46	0.84
1:A:305:PHE:CZ	1:A:522:GLU:HG3	2.12	0.84
1:A:231:GLY:HA2	1:A:233:ASP:OD1	1.78	0.84
1:A:824:VAL:HB	1:A:874:GLU:HG3	1.59	0.84
2:B:824:VAL:CG2	2:B:874:GLU:HG3	2.06	0.83
1:A:132:GLU:C	1:A:134:ASP:HB2	1.99	0.82
1:A:416:GLN:O	1:A:416:GLN:HG3	1.81	0.81
2:B:904:ARG:NH2	2:B:921:GLN:HB3	1.96	0.80
1:A:816:ARG:HD3	1:A:868:ASP:OD1	1.80	0.80
1:A:238:MET:CE	1:A:450:ILE:HG21	2.13	0.79
2:B:409:THR:HG23	2:B:419:ILE:HD13	1.63	0.79
1:A:242:MET:HE2	1:A:384:VAL:HG11	1.64	0.79
1:A:323:LEU:O	1:A:324:GLU:HB2	1.83	0.78
1:A:253:GLU:HG2	1:A:313:HIS:HB3	1.65	0.77
1:A:331:ILE:HD12	1:A:667:PHE:HE1	1.50	0.77
1:A:114:LEU:HD11	1:A:476:LYS:CG	2.16	0.76
2:B:335:ARG:NH2	2:B:377:GLY:HA3	2.01	0.76
2:B:335:ARG:NH2	2:B:377:GLY:HA2	2.00	0.76
1:A:825:TYR:CD2	1:A:844:ARG:HD2	2.21	0.75
2:B:106:HIS:HD2	2:B:123:LEU:HD12	1.50	0.75
2:B:458:HIS:HB2	4:B:2131:HOH:O	1.87	0.75
1:A:176:THR:H	1:A:416:GLN:NE2	1.85	0.75
1:A:126:SER:HB3	1:A:131:THR:OG1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:GLU:HG3	1:A:880:GLY:HA3	1.69	0.74
2:B:904:ARG:NH2	2:B:921:GLN:CB	2.51	0.73
2:B:653:ARG:HD2	4:B:2223:HOH:O	1.88	0.73
2:B:560[B]:ARG:HG3	2:B:560[B]:ARG:NH1	1.93	0.72
1:A:331:ILE:CD1	1:A:667:PHE:HE1	2.02	0.72
1:A:882:TRP:O	1:A:886:GLN:HG3	1.89	0.72
1:A:86:ASN:HB3	2:B:87:VAL:HG21	1.71	0.72
1:A:176:THR:H	1:A:416:GLN:HE22	1.38	0.71
1:A:230:GLU:O	1:A:261:ARG:NH2	2.23	0.71
1:A:915:MET:HE3	1:A:919:GLN:HG3	1.71	0.71
1:A:816:ARG:CD	1:A:868:ASP:OD1	2.38	0.70
2:B:88:LYS:O	2:B:92:VAL:HG12	1.91	0.70
1:A:729:HIS:HE1	4:A:2213:HOH:O	1.73	0.70
2:B:271:LEU:CD1	2:B:316:LEU:HD22	2.21	0.70
1:A:519:VAL:HG12	1:A:519:VAL:O	1.91	0.70
2:B:261:ARG:HH12	2:B:390:ASN:HD21	1.39	0.69
1:A:171:GLU:O	1:A:174:HIS:HE1	1.75	0.69
1:A:214:GLU:HG2	1:A:230:GLU:HG3	1.73	0.69
1:A:331:ILE:CD1	1:A:667:PHE:CE1	2.75	0.69
2:B:613:LEU:HB3	2:B:654:VAL:HG12	1.73	0.69
2:B:484:ARG:NH2	4:B:2135:HOH:O	2.25	0.68
1:A:470:GLN:N	1:A:471:PRO:CD	2.56	0.68
2:B:560[B]:ARG:NH1	2:B:560[B]:ARG:CG	2.47	0.68
1:A:238:MET:HE2	1:A:450:ILE:HG21	1.75	0.68
2:B:261:ARG:NH1	2:B:390:ASN:HD21	1.92	0.68
2:B:343:GLU:HG3	2:B:348:LYS:HE2	1.75	0.67
1:A:153:LEU:CD1	1:A:153:LEU:C	2.62	0.67
1:A:739:GLN:NE2	2:B:739:GLN:NE2	2.43	0.67
2:B:824:VAL:HG22	2:B:874:GLU:CG	2.17	0.66
1:A:124:ASP:N	1:A:125:PRO:CD	2.59	0.66
2:B:778:PRO:HB2	2:B:781:LEU:HB2	1.77	0.66
1:A:416:GLN:O	1:A:416:GLN:CG	2.43	0.66
1:A:904:ARG:HH22	1:A:921:GLN:HB2	1.59	0.65
1:A:904:ARG:NH1	1:A:922:GLN:OE1	2.29	0.65
2:B:874:GLU:O	2:B:904:ARG:HG3	1.97	0.65
1:A:590:LEU:HB3	1:A:788:VAL:HG12	1.77	0.65
1:A:590:LEU:CB	1:A:788:VAL:CG1	2.74	0.65
1:A:185:GLN:O	1:A:189:GLU:HB2	1.97	0.65
1:A:331:ILE:HG13	1:A:332:GLY:N	2.12	0.64
2:B:825:TYR:CE2	2:B:844:ARG:HD2	2.33	0.64
1:A:104:HIS:CD2	1:A:171:GLU:HB2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:O	1:A:125:PRO:CD	2.46	0.64
2:B:823:LYS:NZ	2:B:874:GLU:OE2	2.23	0.64
2:B:184:ILE:O	2:B:188:ILE:HG12	1.99	0.63
2:B:904:ARG:HH22	2:B:921:GLN:HB2	1.63	0.63
2:B:89:GLN:O	2:B:92:VAL:HG13	1.98	0.63
2:B:613:LEU:HB3	2:B:654:VAL:CG1	2.29	0.62
2:B:229:LEU:HD21	2:B:235:LEU:HB3	1.80	0.62
1:A:413:LYS:C	1:A:415:VAL:O	2.38	0.62
2:B:626:ARG:NH2	2:B:683:GLU:OE1	2.32	0.62
1:A:519:VAL:CG1	1:A:519:VAL:O	2.47	0.62
1:A:904:ARG:NH2	1:A:921:GLN:CB	2.60	0.62
1:A:875:GLU:HG3	1:A:880:GLY:CA	2.30	0.62
1:A:236:ILE:HB	1:A:237:PRO:CD	2.30	0.62
1:A:86:ASN:HB3	2:B:87:VAL:CG2	2.29	0.62
1:A:778:PRO:HB2	1:A:781:LEU:HB2	1.82	0.61
1:A:331:ILE:HD11	1:A:667:PHE:CE1	2.36	0.61
1:A:509:TYR:HE1	1:A:519:VAL:HG11	1.66	0.61
2:B:342:ASP:O	2:B:344:PRO:HD3	2.00	0.61
1:A:330:VAL:O	1:A:333:SER:HB3	2.00	0.61
2:B:415:VAL:O	2:B:415:VAL:HG13	1.99	0.61
2:B:875:GLU:HG3	2:B:880:GLY:HA3	1.81	0.61
2:B:235:LEU:HD22	2:B:388:ILE:HD11	1.82	0.61
2:B:647:ASN:ND2	4:B:2219:HOH:O	2.34	0.61
2:B:534:SER:N	2:B:535:PRO:CD	2.65	0.60
1:A:590:LEU:HB3	1:A:788:VAL:CG1	2.30	0.60
2:B:271:LEU:HD11	2:B:316:LEU:HD22	1.84	0.60
1:A:509:TYR:CE1	1:A:519:VAL:HG11	2.37	0.60
1:A:754:PRO:O	1:A:757:VAL:HG12	2.02	0.60
1:A:739:GLN:HE22	2:B:739:GLN:NE2	2.00	0.60
2:B:327:SER:N	2:B:328:PRO:HD2	2.17	0.60
2:B:323:LEU:O	2:B:324:GLU:HB2	2.02	0.59
1:A:556[A]:GLU:CD	4:A:2160:HOH:O	2.40	0.59
1:A:887:HIS:HD2	4:A:2308:HOH:O	1.85	0.59
1:A:305:PHE:CE2	1:A:522:GLU:HG3	2.38	0.58
1:A:521:ALA:O	1:A:524:ARG:NH2	2.36	0.58
2:B:904:ARG:HH22	2:B:921:GLN:CB	2.16	0.58
1:A:104:HIS:CE1	1:A:105:GLN:HG3	2.38	0.58
1:A:228:SER:HG	1:A:230:GLU:HG3	1.66	0.58
2:B:872:CYS:HA	2:B:902:ALA:O	2.04	0.58
1:A:547:ASN:ND2	1:A:547:ASN:H	2.02	0.58
1:A:202:ARG:O	1:A:206:GLU:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:ALA:C	1:A:788:VAL:HG23	2.24	0.58
1:A:564:VAL:HG21	1:A:570:MET:CE	2.34	0.58
1:A:484:ARG:NH1	4:A:2121:HOH:O	2.36	0.58
2:B:335:ARG:HH22	2:B:377:GLY:CA	2.15	0.57
1:A:473:MET:O	1:A:476:LYS:HB2	2.04	0.57
2:B:784:HIS:CE1	2:B:786:LEU:HB2	2.39	0.57
1:A:214:GLU:CG	1:A:228:SER:OG	2.52	0.57
1:A:590:LEU:HB2	1:A:788:VAL:CG1	2.34	0.57
1:A:547:ASN:H	1:A:547:ASN:HD22	1.53	0.57
1:A:498:THR:HB	4:A:2126:HOH:O	2.05	0.57
1:A:122:ASP:O	1:A:125:PRO:HD2	2.05	0.57
1:A:327:SER:N	1:A:328:PRO:HD2	2.20	0.56
1:A:407:TYR:HD1	1:A:408:CYS:N	1.98	0.56
1:A:823:LYS:NZ	1:A:874:GLU:OE2	2.29	0.56
1:A:854:LYS:O	1:A:857:GLN:HG3	2.05	0.56
2:B:138:THR:HG22	2:B:152:LYS:HG2	1.87	0.56
1:A:872:CYS:HA	1:A:902:ALA:O	2.05	0.56
2:B:626:ARG:HH22	2:B:683:GLU:CD	2.07	0.56
1:A:739:GLN:NE2	2:B:739:GLN:HE22	2.04	0.56
1:A:556[A]:GLU:OE2	4:A:2160:HOH:O	2.18	0.56
1:A:659:LEU:CD1	2:B:359:ALA:HA	2.35	0.55
1:A:221:PHE:O	1:A:223:GLY:N	2.36	0.55
2:B:875:GLU:HG3	2:B:880:GLY:CA	2.35	0.55
2:B:345:SER:O	2:B:348:LYS:HB2	2.07	0.55
2:B:876:PRO:HA	2:B:904:ARG:HB2	1.87	0.55
1:A:214:GLU:HG2	1:A:230:GLU:CG	2.37	0.55
1:A:340:ARG:HD2	4:A:2049:HOH:O	2.07	0.54
1:A:231:GLY:CA	1:A:233:ASP:OD1	2.52	0.54
1:A:564:VAL:HG21	1:A:570:MET:HE1	1.88	0.54
2:B:343:GLU:OE1	2:B:348:LYS:CE	2.55	0.54
2:B:844:ARG:HD3	4:B:2332:HOH:O	2.06	0.54
1:A:825:TYR:CE2	1:A:844:ARG:HD2	2.42	0.54
1:A:124:ASP:H	1:A:125:PRO:HD3	1.71	0.54
2:B:904:ARG:NH2	2:B:921:GLN:HB2	2.21	0.54
2:B:345:SER:OG	2:B:347:ASN:OD1	2.25	0.54
2:B:825:TYR:CG	2:B:844:ARG:HD2	2.42	0.54
1:A:526:MET:CE	1:A:530:SER:HB3	2.38	0.54
2:B:547:ASN:H	2:B:547:ASN:HD22	1.56	0.53
2:B:305:PHE:CE2	2:B:522:GLU:HG3	2.42	0.53
1:A:420:PHE:CE1	1:A:436:LEU:HD23	2.43	0.53
1:A:613:LEU:HD23	1:A:654:VAL:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLU:HG2	4:A:2127:HOH:O	2.07	0.53
1:A:825:TYR:CG	1:A:844:ARG:HD2	2.44	0.53
1:A:331:ILE:HD11	1:A:667:PHE:CD1	2.43	0.53
2:B:426:ASP:C	2:B:426:ASP:OD1	2.46	0.53
2:B:893:ILE:HB	2:B:894:PRO:CD	2.39	0.53
1:A:325:ILE:HG13	1:A:325:ILE:O	2.08	0.52
2:B:202:ARG:HD2	4:B:2048:HOH:O	2.09	0.52
2:B:409:THR:HG21	2:B:419:ILE:HG21	1.90	0.52
1:A:710:ARG:NH2	4:A:2226:HOH:O	2.43	0.52
2:B:350:LEU:HD12	2:B:351:PRO:HD2	1.91	0.52
4:A:2235:HOH:O	2:B:707:LYS:HE2	2.10	0.52
2:B:904:ARG:HH21	2:B:921:GLN:HB3	1.75	0.52
1:A:426:ASP:O	1:A:430:VAL:HG23	2.10	0.52
2:B:652:PHE:C	2:B:653:ARG:HG2	2.31	0.51
2:B:498:THR:O	2:B:499:LEU:C	2.49	0.51
2:B:390:ASN:O	2:B:391:GLN:HB2	2.10	0.51
1:A:350:LEU:HD22	1:A:438:LEU:HD11	1.92	0.51
1:A:197:SER:O	1:A:201:LYS:HD3	2.11	0.51
2:B:816:ARG:HD2	2:B:870:VAL:HG23	1.93	0.51
1:A:571:GLN:HE21	1:A:572:SER:H	1.58	0.50
2:B:106:HIS:CD2	2:B:123:LEU:HD12	2.39	0.50
2:B:236:ILE:HB	2:B:237:PRO:CD	2.41	0.50
1:A:124:ASP:N	1:A:125:PRO:HD3	2.25	0.50
2:B:407:TYR:C	2:B:409:THR:H	2.16	0.50
2:B:122:ASP:HB2	4:B:2013:HOH:O	2.12	0.50
2:B:388:ILE:O	2:B:388:ILE:HG22	2.12	0.49
1:A:214:GLU:HG3	1:A:228:SER:OG	2.13	0.49
1:A:378:TYR:HH	1:A:614:SER:HG	1.59	0.49
2:B:206:GLU:HG2	2:B:240:LYS:HD3	1.93	0.49
1:A:590:LEU:CB	1:A:788:VAL:HG12	2.40	0.49
2:B:325:ILE:HD13	2:B:365:VAL:HG11	1.93	0.49
1:A:305:PHE:CZ	1:A:522:GLU:CG	2.90	0.49
2:B:351:PRO:HB2	2:B:383:THR:HB	1.93	0.49
1:A:144:PHE:CE2	1:A:160:LEU:HD23	2.47	0.49
1:A:357:ASP:O	1:A:360:VAL:HG12	2.13	0.49
2:B:607:GLU:HG3	2:B:607:GLU:O	2.12	0.49
2:B:242:MET:CE	2:B:386:ILE:HD11	2.43	0.49
1:A:656:ASP:O	1:A:657:SER:O	2.30	0.49
2:B:261:ARG:HH12	2:B:390:ASN:ND2	2.10	0.48
1:A:131:THR:O	1:A:132:GLU:CG	2.62	0.48
1:A:556[B]:GLU:CG	1:A:560:ARG:HH21	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:GLU:CG	2:B:348:LYS:HE2	2.42	0.48
1:A:470:GLN:N	1:A:471:PRO:HD3	2.28	0.48
1:A:236:ILE:CB	1:A:237:PRO:HD3	2.38	0.47
1:A:331:ILE:HD12	1:A:667:PHE:CE1	2.36	0.47
1:A:656:ASP:C	1:A:657:SER:O	2.52	0.47
2:B:526:MET:HG3	4:B:2153:HOH:O	2.13	0.47
2:B:214:GLU:HG2	2:B:230:GLU:HG3	1.97	0.47
2:B:885:SER:O	2:B:886:GLN:C	2.53	0.47
1:A:534:SER:N	1:A:535:PRO:CD	2.78	0.47
1:A:816:ARG:HD2	1:A:868:ASP:OD1	2.14	0.47
2:B:171:GLU:HG3	2:B:419:ILE:HB	1.96	0.47
1:A:787:ALA:C	1:A:788:VAL:CG2	2.82	0.47
1:A:564:VAL:HG11	1:A:570:MET:HE2	1.96	0.47
2:B:343:GLU:OE1	2:B:348:LYS:HE3	2.15	0.47
2:B:456:ARG:NH1	4:B:2131:HOH:O	2.48	0.47
2:B:816:ARG:HG3	2:B:817:VAL:N	2.29	0.47
1:A:273:LYS:NZ	1:A:281:GLU:OE1	2.48	0.47
1:A:176:THR:N	1:A:416:GLN:HE22	2.11	0.47
1:A:368:GLU:OE1	1:A:662:GLU:HB3	2.15	0.47
1:A:214:GLU:CG	1:A:230:GLU:HG3	2.44	0.47
1:A:413:LYS:O	1:A:415:VAL:O	2.33	0.47
2:B:533:TRP:CH2	2:B:676:PRO:HB3	2.50	0.46
1:A:584:MET:HA	1:A:589:LYS:O	2.16	0.46
2:B:350:LEU:HD22	2:B:438:LEU:HD21	1.97	0.46
1:A:653:ARG:HD2	4:A:2180:HOH:O	2.16	0.46
2:B:153:LEU:C	2:B:155:GLU:H	2.19	0.46
1:A:915:MET:HE3	1:A:919:GLN:CG	2.42	0.46
1:A:372:MET:C	1:A:374:LYS:H	2.19	0.46
1:A:834:LYS:HB2	1:A:834:LYS:HE3	1.60	0.46
2:B:271:LEU:CD1	2:B:316:LEU:CD2	2.93	0.46
1:A:526:MET:HE2	1:A:530:SER:HB3	1.98	0.46
1:A:923:GLN:NE2	1:A:927:ASN:OD1	2.49	0.46
1:A:214:GLU:HG2	1:A:228:SER:OG	2.16	0.46
1:A:334:VAL:HG22	1:A:380:VAL:HG11	1.97	0.46
2:B:89:GLN:O	2:B:92:VAL:CG1	2.63	0.46
1:A:122:ASP:O	1:A:125:PRO:HD3	2.15	0.46
1:A:644:HIS:HE1	4:A:2192:HOH:O	1.99	0.46
2:B:204:LEU:O	2:B:208:THR:OG1	2.28	0.45
1:A:849:TYR:HA	1:A:850:PRO:C	2.35	0.45
1:A:171:GLU:HG2	1:A:171:GLU:O	2.15	0.45
1:A:357:ASP:HB2	4:A:2093:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:MET:HE3	2:B:386:ILE:HD11	1.98	0.45
1:A:533:TRP:CH2	1:A:676:PRO:HB3	2.51	0.45
2:B:409:THR:HG23	2:B:419:ILE:CD1	2.40	0.45
2:B:778:PRO:CB	2:B:781:LEU:HB2	2.46	0.45
1:A:840:VAL:O	1:A:840:VAL:HG13	2.15	0.45
1:A:206:GLU:OE2	1:A:240:LYS:HE3	2.16	0.45
1:A:221:PHE:C	1:A:223:GLY:H	2.20	0.45
1:A:327:SER:O	1:A:331:ILE:HG23	2.16	0.45
1:A:556[B]:GLU:HG3	1:A:560:ARG:HH21	1.81	0.45
1:A:343:GLU:HA	1:A:344:PRO:HD3	1.63	0.45
2:B:343:GLU:OE1	2:B:348:LYS:HE2	2.17	0.45
2:B:652:PHE:CE1	2:B:654:VAL:HG22	2.52	0.45
1:A:420:PHE:CE1	1:A:436:LEU:CD2	3.00	0.45
2:B:214:GLU:HG2	2:B:228:SER:OG	2.17	0.45
2:B:644:HIS:HE1	4:B:2214:HOH:O	2.00	0.45
2:B:904:ARG:NH1	2:B:922:GLN:OE1	2.50	0.45
2:B:686:PHE:CZ	2:B:729:HIS:HD2	2.35	0.45
2:B:327:SER:HB2	2:B:328:PRO:HD3	1.99	0.44
1:A:837:GLN:HG2	1:A:839:ASP:OD1	2.18	0.44
2:B:331:ILE:HD11	2:B:383:THR:HG21	1.98	0.44
2:B:704:GLY:HA3	4:B:2231:HOH:O	2.17	0.44
1:A:421:HIS:HA	1:A:451:ASP:HB3	2.00	0.44
2:B:242:MET:HB2	2:B:242:MET:HE2	1.79	0.44
1:A:89:GLN:HE21	1:A:93:LEU:HD23	1.82	0.44
2:B:335:ARG:HH22	2:B:377:GLY:HA3	1.73	0.44
1:A:238:MET:HE1	1:A:450:ILE:HG21	1.96	0.44
2:B:227:PHE:CD2	2:B:260:HIS:HD2	2.35	0.44
2:B:668:GLU:OE1	2:B:668:GLU:HA	2.17	0.44
1:A:659:LEU:HD13	2:B:359:ALA:HA	2.00	0.44
2:B:319:ASN:HB3	2:B:326:VAL:HG21	2.00	0.44
1:A:904:ARG:HH21	1:A:921:GLN:CB	2.29	0.44
2:B:320:PRO:HD3	2:B:700:PHE:CZ	2.53	0.44
1:A:175:ILE:HD11	1:A:418:PRO:HD3	1.99	0.43
1:A:409:THR:HB	1:A:419:ILE:HD13	1.99	0.43
2:B:811:PRO:HG3	2:B:862:GLN:HE21	1.83	0.43
1:A:887:HIS:CD2	4:A:2308:HOH:O	2.67	0.43
2:B:137:GLU:HG2	4:B:2023:HOH:O	2.18	0.43
1:A:228:SER:OG	1:A:230:GLU:CG	2.50	0.43
1:A:319:ASN:HB2	1:A:320:PRO:HD2	2.01	0.43
1:A:599:LEU:O	1:A:603:THR:HG23	2.19	0.43
2:B:609:ILE:HA	2:B:610:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:TYR:CD1	1:A:407:TYR:C	2.89	0.43
1:A:407:TYR:HD1	1:A:407:TYR:C	2.21	0.43
1:A:556[B]:GLU:HA	1:A:556[B]:GLU:OE1	2.18	0.43
1:A:923:GLN:HE21	1:A:927:ASN:CG	2.22	0.43
2:B:823:LYS:HE2	2:B:823:LYS:HB2	1.84	0.43
2:B:547:ASN:ND2	2:B:547:ASN:H	2.16	0.43
2:B:886:GLN:NE2	2:B:890:ARG:HH11	2.16	0.43
1:A:851:PHE:HA	1:A:852:PRO:HD3	1.69	0.43
1:A:545:TYR:HB3	1:A:767:ARG:HB2	2.00	0.43
2:B:613:LEU:HD13	2:B:654:VAL:CG1	2.49	0.43
1:A:564:VAL:CG2	1:A:570:MET:HE1	2.49	0.43
1:A:196:ASN:C	1:A:196:ASN:OD1	2.58	0.43
2:B:204:LEU:HG	2:B:505:MET:SD	2.58	0.42
1:A:763:ARG:O	1:A:767:ARG:HB3	2.19	0.42
1:A:823:LYS:HE2	1:A:823:LYS:HB2	1.86	0.42
2:B:261:ARG:CD	2:B:456:ARG:NH2	2.82	0.42
2:B:849:TYR:HA	2:B:850:PRO:C	2.39	0.42
1:A:523:TRP:CH2	1:A:525:PRO:HG3	2.54	0.42
2:B:824:VAL:HG21	4:B:2347:HOH:O	2.19	0.42
1:A:122:ASP:C	1:A:124:ASP:H	2.22	0.42
2:B:327:SER:N	2:B:328:PRO:CD	2.82	0.42
1:A:793:GLU:HG2	4:A:2267:HOH:O	2.19	0.42
2:B:507:ASN:OD1	2:B:510:ARG:NH2	2.51	0.42
1:A:144:PHE:CE2	1:A:160:LEU:CD2	3.03	0.42
1:A:904:ARG:HH21	1:A:921:GLN:HB2	1.78	0.42
2:B:175:ILE:HG22	2:B:177:SER:H	1.85	0.42
2:B:734:LEU:HG	2:B:738:LEU:CD2	2.50	0.42
1:A:747:GLN:HA	1:A:849:TYR:O	2.19	0.42
2:B:893:ILE:CB	2:B:894:PRO:CD	2.98	0.42
2:B:703:SER:HB2	2:B:707:LYS:HD2	2.02	0.42
1:A:126:SER:O	1:A:129:ASP:N	2.52	0.42
2:B:613:LEU:HD13	2:B:654:VAL:HG12	2.02	0.42
2:B:556:GLU:HG2	4:B:2186:HOH:O	2.18	0.42
2:B:146:SER:OG	2:B:147:GLY:HA2	2.20	0.42
1:A:331:ILE:CD1	1:A:667:PHE:CD1	3.03	0.41
2:B:231:GLY:O	2:B:454:CYS:HB2	2.20	0.41
1:A:766:LEU:HD23	1:A:766:LEU:HA	1.74	0.41
2:B:628:ALA:O	2:B:640:THR:HG23	2.20	0.41
1:A:710:ARG:HD3	1:A:710:ARG:HA	1.87	0.41
1:A:111:PRO:HB3	1:A:425:ASP:OD2	2.21	0.41
1:A:176:THR:N	1:A:416:GLN:NE2	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:LEU:HD11	2:B:316:LEU:HB2	2.00	0.41
1:A:781:LEU:HD21	1:A:826:TYR:CD1	2.56	0.41
1:A:593:TRP:CZ2	1:A:778:PRO:HG3	2.55	0.41
1:A:694:GLN:HG2	2:B:694:GLN:HG2	2.03	0.41
1:A:552:LYS:O	1:A:556[A]:GLU:HG3	2.20	0.41
2:B:485:LYS:HD3	2:B:485:LYS:HA	1.85	0.41
1:A:91:LYS:CD	1:A:94:GLN:OE1	2.69	0.41
1:A:236:ILE:CB	1:A:237:PRO:CD	2.95	0.41
2:B:102:ARG:O	2:B:105:GLN:HG3	2.21	0.41
1:A:407:TYR:O	1:A:410:ASP:HB2	2.21	0.41
1:A:331:ILE:HG13	1:A:332:GLY:H	1.84	0.41
1:A:820:CYS:O	1:A:844:ARG:HA	2.20	0.41
1:A:91:LYS:HE3	1:A:130:LEU:HD12	2.03	0.41
2:B:298:HIS:HB3	2:B:319:ASN:O	2.21	0.40
2:B:915:MET:HE3	2:B:919:GLN:HG3	2.02	0.40
2:B:551:MET:O	2:B:552:LYS:C	2.59	0.40
2:B:335:ARG:HH22	2:B:377:GLY:HA2	1.78	0.40
1:A:473:MET:HG3	1:A:474:TYR:N	2.36	0.40
2:B:415:VAL:O	2:B:416:GLN:HB3	2.22	0.40
2:B:204:LEU:HD22	2:B:491:LEU:HD12	2.03	0.40
2:B:233:ASP:N	2:B:233:ASP:OD1	2.54	0.40
2:B:257:GLY:HA2	4:B:2062:HOH:O	2.21	0.40
1:A:526:MET:HE3	1:A:530:SER:HB3	2.02	0.40
2:B:86:ASN:ND2	4:B:2001:HOH:O	2.54	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	796/933 (85%)	737 (93%)	51 (6%)	8 (1%)	19 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	795/933 (85%)	749 (94%)	45 (6%)	1 (0%)	56 81
All	All	1591/1866 (85%)	1486 (93%)	96 (6%)	9 (1%)	30 56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	657	SER
1	A	659	LEU
1	A	344	PRO
1	A	172	TYR
1	A	324	GLU
2	B	886	GLN
1	A	222	PRO
1	A	415	VAL
1	A	103	GLY

### 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	650/789 (82%)	605 (93%)	45 (7%)	19 38
2	B	639/789 (81%)	593 (93%)	46 (7%)	18 35
All	All	1289/1578 (82%)	1198 (93%)	91 (7%)	18 36

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ASP
1	A	138	THR
1	A	153	LEU
1	A	190	SER
1	A	201	LYS
1	A	205	SER
1	A	206	GLU

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Mol	Chain	Res	Type
1	A	214	GLU
1	A	220	LYS
1	A	233	ASP
1	A	261	ARG
1	A	265	ASN
1	A	271	LEU
1	A	285	LYS
1	A	327	SER
1	A	331	ILE
1	A	334	VAL
1	A	407	TYR
1	A	410	ASP
1	A	414	MET
1	A	419	ILE
1	A	457	ARG
1	A	473	MET
1	A	484	ARG
1	A	504	GLU
1	A	547	ASN
1	A	571	GLN
1	A	576	LYS
1	A	616	GLU
1	A	633	GLN
1	A	647	ASN
1	A	654	VAL
1	A	657	SER
1	A	661	GLU
1	A	688	ASP
1	A	725	GLN
1	A	739	GLN
1	A	767	ARG
1	A	816	ARG
1	A	821	SER
1	A	834	LYS
1	A	860	LEU
1	A	877	LEU
1	A	900	ARG
1	A	932	VAL
2	B	92	VAL
2	B	122	ASP
2	B	132	GLU
2	B	138	THR

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Mol	Chain	Res	Type
2	B	149	GLU
2	B	171	GLU
2	B	179	GLU
2	B	228	SER
2	B	233	ASP
2	B	252	ARG
2	B	265	ASN
2	B	278	LEU
2	B	311	LEU
2	B	335	ARG
2	B	340	ARG
2	B	343	GLU
2	B	361	THR
2	B	373	SER
2	B	379	GLU
2	B	383	THR
2	B	409	THR
2	B	415	VAL
2	B	438	LEU
2	B	445	LYS
2	B	456	ARG
2	B	479	LYS
2	B	485	LYS
2	B	499	LEU
2	B	537	LEU
2	B	547	ASN
2	B	556	GLU
2	B	613	LEU
2	B	620	ARG
2	B	653	ARG
2	B	654	VAL
2	B	657	SER
2	B	688	ASP
2	B	738	LEU
2	B	739	GLN
2	B	777	SER
2	B	786	LEU
2	B	809	LEU
2	B	816	ARG
2	B	824	VAL
2	B	892	VAL
2	B	900	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	117	GLN
1	A	174	HIS
1	A	322	HIS
1	A	416	GLN
1	A	480	HIS
1	A	547	ASN
1	A	571	GLN
1	A	582	GLN
1	A	644	HIS
1	A	739	GLN
1	A	887	HIS
1	A	923	GLN
2	B	106	HIS
2	B	260	HIS
2	B	390	ASN
2	B	529	HIS
2	B	547	ASN
2	B	582	GLN
2	B	598	ASN
2	B	644	HIS
2	B	739	GLN
2	B	862	GLN
2	B	886	GLN
2	B	887	HIS
2	B	888	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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AMP	A	1934	-	20,25,25	1.12	2 (10%)	22,38,38	2.11	4 (18%)
3	AMP	B	1934	-	20,25,25	1.11	2 (10%)	22,38,38	1.97	4 (18%)

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	AMP	A	1934	-	-	0/6/26/26	0/3/3/3
3	AMP	B	1934	-	-	0/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1934	AMP	C2-N3	2.02	1.35	1.32
3	B	1934	AMP	C2-N3	2.47	1.36	1.32
3	B	1934	AMP	C5-C4	2.76	1.46	1.40
3	A	1934	AMP	C5-C4	2.95	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1934	AMP	N3-C2-N1	-6.72	123.75	128.89
3	A	1934	AMP	N3-C2-N1	-6.54	123.88	128.89
3	A	1934	AMP	C2'-C1'-N9	-5.25	106.27	114.29
3	B	1934	AMP	C2'-C1'-N9	-3.43	109.05	114.29
3	B	1934	AMP	C4-C5-N7	-2.61	107.08	109.48
3	A	1934	AMP	C4-C5-N7	-2.41	107.26	109.48
3	A	1934	AMP	O3'-C3'-C2'	-2.35	104.17	111.83
3	B	1934	AMP	O3'-C3'-C2'	-2.07	105.11	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	812/933 (87%)	-0.43	15 (1%) 71 66	11, 29, 67, 100	0
2	B	807/933 (86%)	-0.49	12 (1%) 76 71	10, 27, 65, 88	0
All	All	1619/1866 (86%)	-0.46	27 (1%) 73 68	10, 28, 66, 100	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	PHE	4.4
1	A	473	MET	4.3
2	B	475	GLN	3.9
1	A	131	THR	3.8
2	B	933	GLU	3.6
1	A	407	TYR	3.5
2	B	474	TYR	3.4
2	B	343	GLU	3.1
1	A	114	LEU	3.1
1	A	342	ASP	3.1
1	A	116	GLN	2.8
1	A	471	PRO	2.8
2	B	222	PRO	2.8
2	B	113	GLY	2.5
1	A	634	SER	2.5
2	B	147	GLY	2.5
2	B	647	ASN	2.5
1	A	129	ASP	2.4
1	A	125	PRO	2.3
1	A	470	GLN	2.3
2	B	632	ASN	2.3
1	A	136	GLN	2.3
2	B	391	GLN	2.2
2	B	115	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	474	TYR	2.1
2	B	149	GLU	2.0
1	A	895	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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( $\text{\AA}^2$ )	Q<0.9
3	AMP	A	1934	23/23	0.98	0.11	-0.40	6,18,29,29	0
3	AMP	B	1934	23/23	0.98	0.09	-0.53	4,19,29,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.