



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:44 PM GMT

PDB ID : 1GZ4
Title : MOLECULAR MECHANISM OF THE REGULATION OF HUMAN MITOCHONDRIAL NAD(P)⁺-DEPENDENT MALIC ENZYME BY ATP AND FUMARATE
Authors : Yang, Z.; Lanks, C.W.; Tong, L.
Deposited on : 2002-05-15
Resolution : 2.20 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

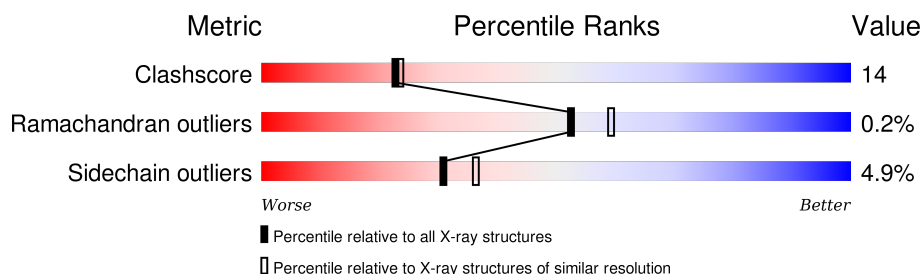
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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	A	551	
1	B	551	
1	C	551	
1	D	551	

2 Entry composition [i](#)

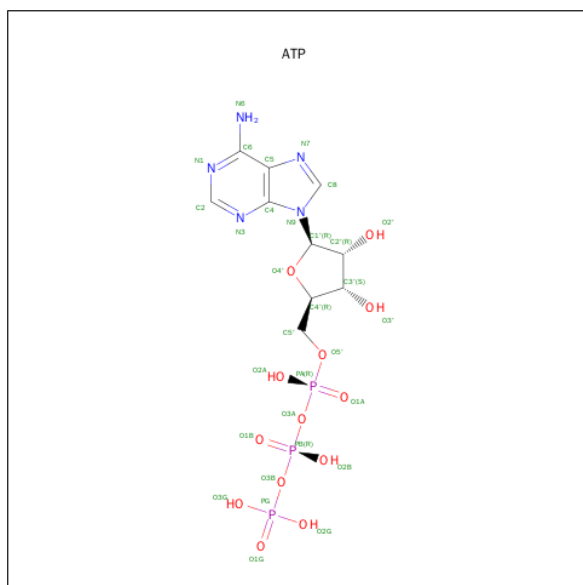
There are 6 unique types of molecules in this entry. The entry contains 18289 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD-DEPENDENT MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	Se	0	0	0
			4350	2784	741	802	9	14			
1	B	551	Total	C	N	O	S	Se	0	0	0
			4350	2784	741	802	9	14			
1	C	551	Total	C	N	O	S	Se	0	0	0
			4350	2784	741	802	9	14			
1	D	551	Total	C	N	O	S	Se	0	0	0
			4351	2784	741	803	9	14			

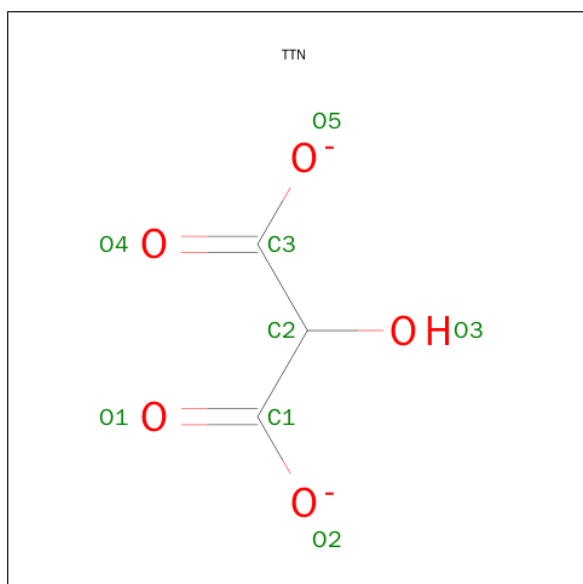
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is TARTRONATE (three-letter code: TTN) (formula: $C_3H_2O_5$).

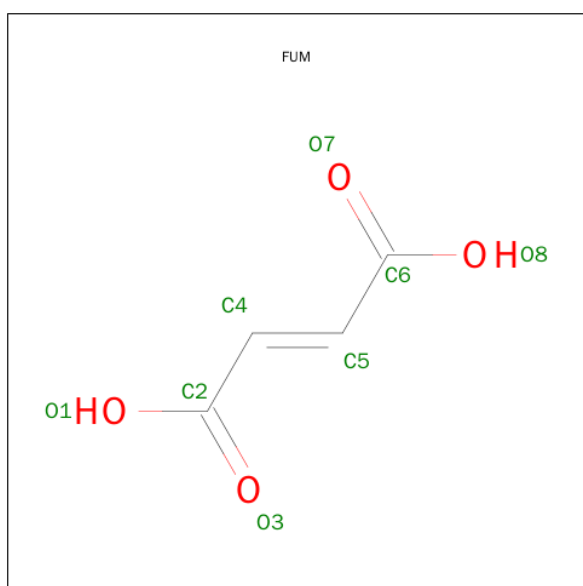


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	3	5		
3	B	1	Total	C	O	0	0
			8	3	5		
3	C	1	Total	C	O	0	0
			8	3	5		
3	D	1	Total	C	O	0	0
			8	3	5		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mn 1 1	0	0
4	A	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 4 4	0	0
5	B	1	Total C O 8 4 4	0	0
5	C	1	Total C O 8 4 4	0	0
5	D	1	Total C O 8 4 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	150	Total O 150 150	0	0
6	B	142	Total O 142 142	0	0

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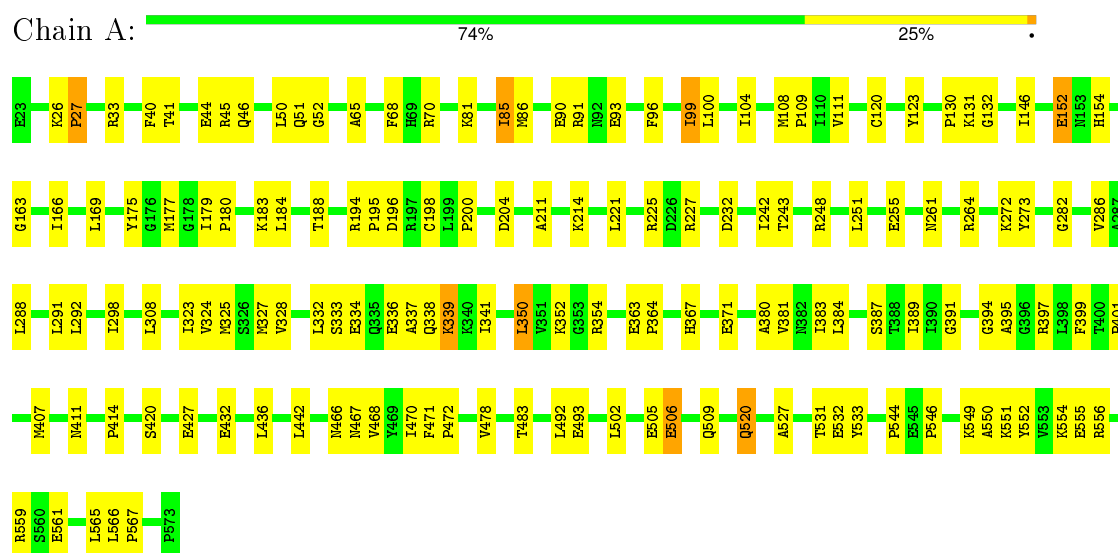
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	130	Total	O	0	0
			130	130		
6	D	150	Total	O	0	0
			150	150		

3 Residue-property plots

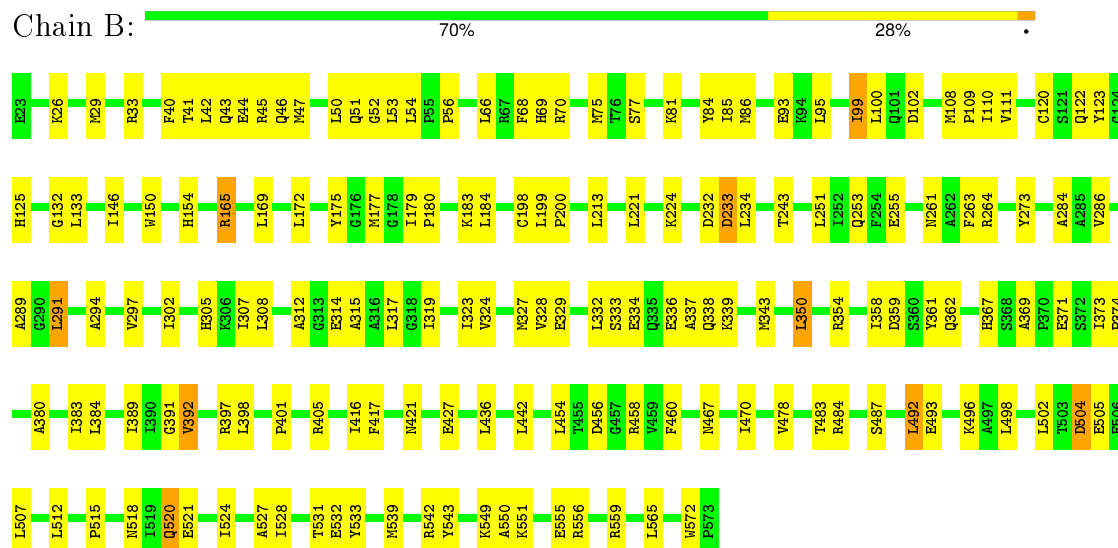
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

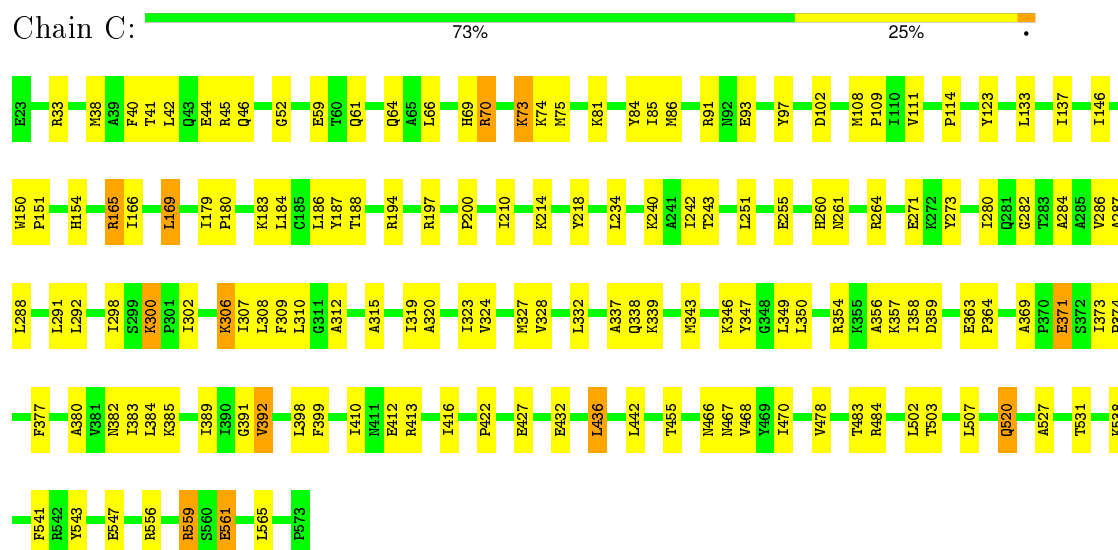
• Molecule 1: NAD-DEPENDENT MALIC ENZYME



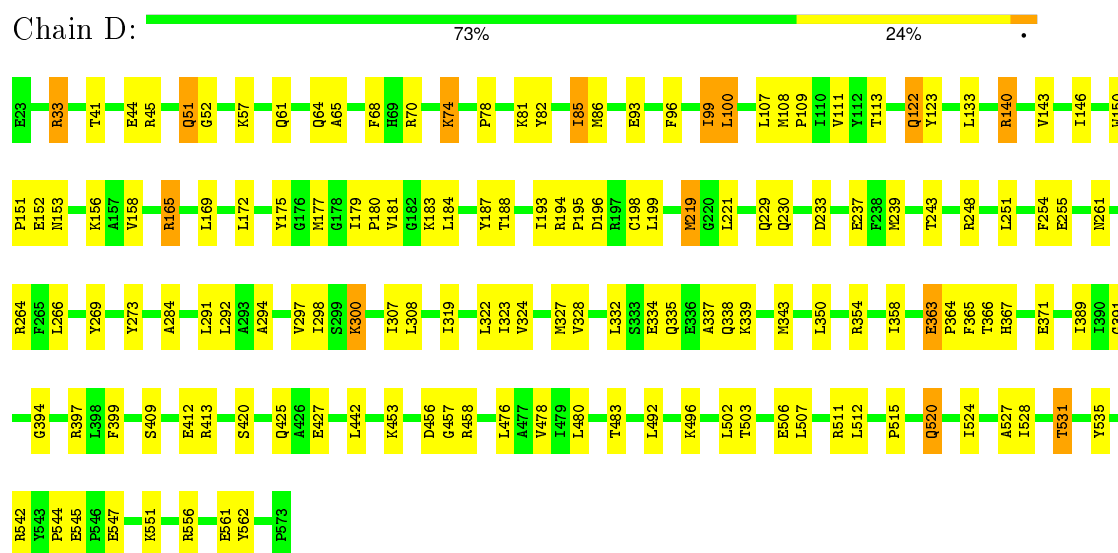
• Molecule 1: NAD-DEPENDENT MALIC ENZYME



• Molecule 1: NAD-DEPENDENT MALIC ENZYME



• Molecule 1: NAD-DEPENDENT MALIC ENZYME



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.94Å 117.45Å 111.61Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	95.0 (20.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18289	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

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: FUM, TTN, ATP, MN

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	0.36	0/4430	0.58	0/5976
1	B	0.35	0/4430	0.60	0/5976
1	C	0.35	0/4430	0.60	1/5976 (0.0%)
1	D	0.35	0/4431	0.59	0/5976
All	All	0.35	0/17721	0.59	1/23904 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	ARG	NE-CZ-NH2	-6.08	117.26	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4350	0	4383	107	0
1	B	4350	0	4383	137	0
1	C	4350	0	4383	122	0
1	D	4351	0	4383	123	0
2	A	62	0	24	0	0
2	B	62	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	62	0	24	1	0
2	D	62	0	24	0	0
3	A	8	0	1	1	0
3	B	8	0	1	1	0
3	C	8	0	1	1	0
3	D	8	0	1	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	8	0	2	1	0
5	B	8	0	2	0	0
5	C	8	0	2	0	0
5	D	8	0	2	0	0
6	A	150	0	0	6	0
6	B	142	0	0	3	0
6	C	130	0	0	3	0
6	D	150	0	0	4	0
All	All	18289	0	17640	479	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 (479) 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:29:MSE:HE2	1:B:50:LEU:HD22	1.28	1.15
1:B:315:ALA:HB3	1:B:392:VAL:HG21	1.25	1.10
1:A:381:VAL:HG13	1:A:407:MSE:HE3	1.38	1.06
1:C:286:VAL:HG21	1:C:467:ASN:HA	1.39	1.04
1:D:343:MSE:HE2	1:D:365:PHE:HB2	1.41	0.98
1:B:323:ILE:HG22	1:B:327:MSE:HE2	1.42	0.97
1:D:327:MSE:HE3	1:D:337:ALA:HB1	1.46	0.95
1:C:323:ILE:HG22	1:C:327:MSE:HE2	1.49	0.95
1:B:374:PRO:HG3	1:B:383:ILE:HD12	1.49	0.95
1:D:177:MSE:HE2	1:D:181:VAL:HG23	1.47	0.94
1:B:43:GLN:HG2	1:B:47:MSE:HE3	1.48	0.93
1:D:140:ARG:HH22	1:D:233:ASP:HB3	1.33	0.92
1:B:286:VAL:HG21	1:B:467:ASN:HA	1.51	0.92
1:D:177:MSE:HE1	1:D:180:PRO:HB2	1.50	0.92
1:A:286:VAL:HG21	1:A:467:ASN:HA	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ALA:HB1	1:B:373:ILE:HD11	1.51	0.90
1:D:527:ALA:O	1:D:531:THR:HG22	1.71	0.90
1:B:315:ALA:HB3	1:B:392:VAL:CG2	2.03	0.89
1:B:26:LYS:HA	1:B:29:MSE:HE3	1.57	0.86
1:B:315:ALA:CB	1:B:392:VAL:HG21	2.05	0.86
1:D:177:MSE:CE	1:D:180:PRO:HB2	2.07	0.85
1:B:515:PRO:HG2	1:B:518:ASN:HD22	1.40	0.84
1:D:298:ILE:HG22	1:D:300:LYS:HG2	1.59	0.84
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.60	0.83
1:B:66:LEU:HD22	1:B:70:ARG:NH1	1.92	0.82
1:A:381:VAL:CG1	1:A:407:MSE:HE3	2.09	0.82
1:C:184:LEU:HD12	1:C:200:PRO:HG3	1.61	0.82
1:B:334:GLU:O	1:B:338:GLN:HG3	1.78	0.81
1:B:520:GLN:HE21	1:B:520:GLN:H	1.26	0.81
1:B:492:LEU:HD22	1:B:496:LYS:HE3	1.61	0.80
1:A:407:MSE:HE2	1:A:407:MSE:HA	1.63	0.80
1:C:73:LYS:HA	1:C:73:LYS:HE3	1.64	0.80
1:D:323:ILE:HG22	1:D:327:MSE:HE2	1.62	0.79
1:C:286:VAL:CG2	1:C:467:ASN:HA	2.13	0.79
1:B:527:ALA:O	1:B:531:THR:HG23	1.83	0.78
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.66	0.77
1:C:327:MSE:HE3	1:C:337:ALA:HB1	1.67	0.77
1:D:453:LYS:NZ	1:D:457:GLY:HA2	1.99	0.77
1:B:520:GLN:NE2	1:B:520:GLN:H	1.83	0.76
1:C:527:ALA:O	1:C:531:THR:HG23	1.86	0.76
1:A:544:PRO:HD3	1:D:248:ARG:NH1	2.02	0.75
1:A:371:GLU:H	1:A:371:GLU:CD	1.91	0.74
1:C:392:VAL:HG13	1:C:392:VAL:O	1.86	0.74
1:D:177:MSE:O	1:D:177:MSE:HE3	1.88	0.73
1:B:29:MSE:HE2	1:B:50:LEU:CD2	2.15	0.73
1:C:369:ALA:HB1	1:C:373:ILE:HD11	1.70	0.73
1:B:29:MSE:HE1	1:B:53:LEU:HD12	1.71	0.72
1:D:453:LYS:HZ3	1:D:457:GLY:HA2	1.55	0.72
1:B:29:MSE:HE1	1:B:53:LEU:CD1	2.20	0.71
1:C:520:GLN:HE21	1:C:520:GLN:H	1.35	0.71
1:A:85:ILE:HD12	1:A:96:PHE:HE1	1.56	0.70
1:C:183:LYS:HE2	1:C:255:GLU:CD	2.10	0.70
1:D:194:ARG:HH11	1:D:194:ARG:HG2	1.55	0.70
1:C:338:GLN:NE2	1:C:364:PRO:HB3	2.06	0.70
1:D:308:LEU:HB3	1:D:389:ILE:HD12	1.75	0.69
1:B:392:VAL:O	1:B:392:VAL:HG22	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:520:GLN:HE21	1:D:520:GLN:H	1.41	0.68
1:C:520:GLN:NE2	1:C:520:GLN:H	1.90	0.68
1:C:315:ALA:CB	1:C:392:VAL:HG21	2.24	0.68
1:C:354:ARG:CZ	1:C:356:ALA:HB3	2.24	0.68
1:D:456:ASP:OD1	1:D:458:ARG:HD3	1.94	0.68
1:A:81:LYS:O	1:A:85:ILE:HG23	1.92	0.68
1:C:41:THR:OG1	1:C:44:GLU:HG3	1.94	0.67
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.76	0.67
1:B:286:VAL:CG2	1:B:467:ASN:HA	2.25	0.67
1:D:332:LEU:HD12	1:D:332:LEU:H	1.59	0.67
1:D:183:LYS:HE3	1:D:255:GLU:CD	2.15	0.67
1:A:211:ALA:HA	1:A:214:LYS:HE2	1.76	0.67
1:D:179:ILE:HB	1:D:180:PRO:HD3	1.78	0.66
1:B:33:ARG:HD3	1:B:93:GLU:OE2	1.96	0.66
1:D:248:ARG:HH11	1:D:248:ARG:HG2	1.60	0.65
1:A:493:GLU:HG3	1:A:533:TYR:CD1	2.32	0.65
1:B:350:LEU:HD22	1:B:354:ARG:CZ	2.26	0.65
1:C:383:ILE:HG22	1:C:384:LEU:HD12	1.79	0.65
1:C:315:ALA:HB3	1:C:392:VAL:HG21	1.79	0.65
1:B:85:ILE:HD11	1:B:111:VAL:HG22	1.78	0.65
1:A:520:GLN:HE21	1:A:520:GLN:H	1.44	0.64
1:A:532:GLU:HG2	1:A:549:LYS:HG3	1.78	0.64
1:D:68:PHE:CD2	1:D:99:ILE:HG13	2.32	0.64
1:C:243:THR:HG21	1:C:273:TYR:CD2	2.33	0.64
1:C:371:GLU:CD	1:C:371:GLU:H	1.99	0.64
1:D:81:LYS:O	1:D:85:ILE:HG23	1.96	0.64
1:D:298:ILE:HD11	1:D:442:LEU:HD12	1.80	0.64
1:D:358:ILE:HD13	1:D:366:THR:HG21	1.80	0.64
1:D:239:MSE:HE1	1:D:254:PHE:HZ	1.61	0.63
1:C:286:VAL:HG21	1:C:467:ASN:CA	2.23	0.63
1:B:308:LEU:HB3	1:B:389:ILE:HD12	1.80	0.63
1:D:300:LYS:HB3	1:D:300:LYS:NZ	2.13	0.63
1:D:308:LEU:HD23	1:D:389:ILE:HD11	1.81	0.63
1:B:154:HIS:HD2	6:B:2058:HOH:O	1.81	0.63
1:A:350:LEU:HD22	1:A:354:ARG:NH1	2.12	0.63
1:B:85:ILE:HD11	1:B:86:MSE:SE	2.48	0.62
1:B:391:GLY:HA3	1:B:427:GLU:HG2	1.81	0.62
1:A:183:LYS:HE3	1:A:255:GLU:CD	2.20	0.62
1:B:308:LEU:HD23	1:B:389:ILE:HD11	1.80	0.62
1:A:286:VAL:CG2	1:A:467:ASN:HA	2.27	0.62
1:C:346:LYS:HE2	1:C:347:TYR:CZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:VAL:HA	1:C:327:MSE:HE3	1.81	0.62
1:C:264:ARG:HG3	6:C:2075:HOH:O	2.00	0.62
1:C:300:LYS:NZ	1:C:300:LYS:HB3	2.14	0.62
1:D:33:ARG:HD2	1:D:93:GLU:OE1	2.00	0.61
1:D:334:GLU:O	1:D:338:GLN:HG3	2.01	0.61
1:B:68:PHE:CD2	1:B:99:ILE:HG12	2.35	0.61
1:C:310:LEU:HD21	1:C:398:LEU:HB2	1.83	0.61
1:A:551:LYS:HG2	1:A:555:GLU:OE2	2.01	0.61
1:C:154:HIS:HD2	6:C:2072:HOH:O	1.84	0.60
1:C:538:LYS:HD2	1:C:538:LYS:N	2.16	0.60
1:C:179:ILE:HB	1:C:180:PRO:HD3	1.82	0.60
1:A:108:MSE:HB3	1:A:109:PRO:HD3	1.84	0.59
1:C:346:LYS:HE2	1:C:347:TYR:CE1	2.37	0.59
1:D:528:ILE:O	1:D:531:THR:HG23	2.02	0.59
1:D:140:ARG:NH2	1:D:233:ASP:HB3	2.11	0.59
1:B:179:ILE:HB	1:B:180:PRO:HD3	1.84	0.59
1:B:286:VAL:HG22	1:B:470:ILE:HG12	1.83	0.59
1:A:352:LYS:HE3	6:A:2093:HOH:O	2.03	0.59
1:B:493:GLU:HG3	1:B:533:TYR:CD1	2.38	0.59
1:B:324:VAL:HA	1:B:327:MSE:HE3	1.85	0.59
1:C:52:GLY:HA3	1:D:146:ILE:HG23	1.83	0.59
1:B:504:ASP:HA	1:B:507:LEU:HD12	1.84	0.59
1:D:298:ILE:CG2	1:D:300:LYS:HG2	2.31	0.59
1:B:85:ILE:C	1:B:85:ILE:HD12	2.23	0.59
1:B:551:LYS:HE2	1:B:555:GLU:OE1	2.03	0.59
1:C:298:ILE:HD11	1:C:442:LEU:HD12	1.84	0.59
1:D:327:MSE:CE	1:D:337:ALA:HB1	2.27	0.59
1:C:354:ARG:NE	1:C:356:ALA:HB3	2.17	0.59
1:D:86:MSE:HE1	1:D:111:VAL:HG23	1.85	0.59
1:A:163:GLY:HA2	1:A:166:ILE:HD11	1.84	0.58
1:C:371:GLU:OE1	1:C:371:GLU:N	2.32	0.58
1:A:132:GLY:CA	1:A:200:PRO:HG2	2.34	0.58
1:C:382:ASN:O	1:C:385:LYS:HD2	2.03	0.58
1:B:359:ASP:OD2	1:B:362:GLN:HG3	2.03	0.58
1:A:327:MSE:CE	1:A:337:ALA:HB1	2.33	0.58
1:D:239:MSE:HE3	1:D:269:TYR:CE1	2.38	0.58
1:D:140:ARG:HD2	6:D:2042:HOH:O	2.03	0.57
1:A:41:THR:O	1:A:45:ARG:HG3	2.04	0.57
1:A:380:ALA:O	1:A:384:LEU:HD13	2.03	0.57
1:D:520:GLN:NE2	1:D:520:GLN:H	2.03	0.57
1:A:33:ARG:HD3	1:A:93:GLU:OE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:SER:OG	1:A:336:GLU:HG2	2.04	0.57
1:A:152:GLU:HG2	1:A:196:ASP:O	2.05	0.57
1:B:122:GLN:HG2	1:B:125:HIS:HB2	1.87	0.56
1:B:327:MSE:HE3	1:B:337:ALA:HB1	1.86	0.56
1:A:41:THR:OG1	1:A:44:GLU:HG3	2.06	0.56
1:B:456:ASP:OD1	1:B:458:ARG:HD3	2.05	0.56
1:B:41:THR:O	1:B:45:ARG:HG3	2.06	0.56
1:B:478:VAL:HG13	1:B:483:THR:HB	1.87	0.56
1:D:65:ALA:HA	1:D:99:ILE:HD11	1.85	0.56
1:B:556:ARG:HH11	1:B:556:ARG:HG3	1.70	0.56
1:D:70:ARG:O	1:D:74:LYS:HE3	2.04	0.56
1:D:350:LEU:HD22	1:D:354:ARG:NH1	2.21	0.56
1:C:327:MSE:CE	1:C:337:ALA:HB1	2.36	0.56
1:B:528:ILE:O	1:B:532:GLU:HG3	2.05	0.56
1:D:551:LYS:HB3	1:D:551:LYS:HZ2	1.71	0.56
1:B:315:ALA:HB2	6:B:2132:HOH:O	2.06	0.56
1:A:520:GLN:NE2	1:A:520:GLN:H	2.03	0.56
1:B:524:ILE:O	1:B:528:ILE:HG13	2.05	0.55
1:B:261:ASN:HD22	1:B:264:ARG:HH11	1.53	0.55
1:A:85:ILE:HG13	1:A:86:MSE:N	2.20	0.55
1:A:391:GLY:HA3	1:A:427:GLU:HG2	1.88	0.55
1:A:334:GLU:O	1:A:338:GLN:HG3	2.05	0.55
1:C:42:LEU:O	1:C:46:GLN:HG3	2.07	0.55
1:A:384:LEU:HD12	1:A:384:LEU:N	2.22	0.54
1:D:343:MSE:HE3	1:D:350:LEU:HD12	1.89	0.54
1:D:307:ILE:HD13	1:D:323:ILE:HD13	1.90	0.54
1:D:335:GLN:O	1:D:339:LYS:HG2	2.07	0.54
1:A:177:MSE:O	1:A:180:PRO:HD2	2.08	0.54
1:C:286:VAL:HG22	1:C:470:ILE:HG12	1.89	0.54
1:D:177:MSE:CE	1:D:181:VAL:HG23	2.30	0.54
1:A:272:LYS:HD2	1:A:273:TYR:CE1	2.41	0.54
1:D:41:THR:O	1:D:45:ARG:HG3	2.07	0.54
1:C:384:LEU:N	1:C:384:LEU:HD12	2.23	0.54
1:D:551:LYS:NZ	1:D:551:LYS:HB3	2.22	0.54
1:A:527:ALA:O	1:A:531:THR:HG23	2.07	0.54
1:C:183:LYS:HE2	1:C:255:GLU:OE2	2.07	0.54
1:A:132:GLY:HA2	1:A:200:PRO:HG2	1.90	0.54
1:C:385:LYS:HG3	1:C:410:ILE:HD13	1.89	0.54
1:D:248:ARG:HG2	1:D:248:ARG:NH1	2.23	0.53
1:C:338:GLN:HE22	1:C:364:PRO:HB3	1.73	0.53
1:C:243:THR:HG21	1:C:273:TYR:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:MSE:HB3	1:D:109:PRO:HD3	1.91	0.53
1:D:184:LEU:HD13	1:D:198:CYS:HB3	1.89	0.53
1:C:86:MSE:SE	1:C:111:VAL:HG23	2.58	0.53
1:D:332:LEU:CD1	1:D:332:LEU:H	2.22	0.53
1:D:61:GLN:HA	1:D:64:GLN:HE21	1.73	0.53
1:B:333:SER:H	1:B:336:GLU:HG2	1.73	0.53
1:B:183:LYS:HE3	1:B:255:GLU:CD	2.29	0.53
1:A:363:GLU:HB3	1:A:364:PRO:HD3	1.90	0.53
1:C:302:ILE:HD13	1:C:332:LEU:HD13	1.91	0.53
1:C:194:ARG:NH1	1:C:197:ARG:NH2	2.57	0.52
1:B:46:GLN:HG2	1:B:51:GLN:HG3	1.91	0.52
1:D:177:MSE:HE3	1:D:180:PRO:HB2	1.91	0.52
1:C:357:LYS:O	1:C:358:ILE:HD13	2.08	0.52
1:B:132:GLY:CA	1:B:200:PRO:HG2	2.39	0.52
1:D:339:LYS:HA	1:D:367:HIS:CE1	2.43	0.52
1:B:108:MSE:HB3	1:B:109:PRO:HD3	1.91	0.52
1:A:286:VAL:HG22	1:A:470:ILE:HG12	1.90	0.52
1:A:227:ARG:HG2	1:A:227:ARG:HH11	1.74	0.52
1:D:391:GLY:HA3	1:D:427:GLU:HG2	1.92	0.52
1:D:33:ARG:NH2	1:D:196:ASP:HA	2.23	0.52
1:C:33:ARG:HD3	1:C:93:GLU:OE2	2.10	0.52
1:B:315:ALA:O	1:B:319:ILE:HG13	2.10	0.52
1:C:288:LEU:O	1:C:292:LEU:HD13	2.09	0.52
1:C:306:LYS:HE3	1:C:384:LEU:O	2.10	0.51
1:D:86:MSE:CE	1:D:111:VAL:HG23	2.40	0.51
1:D:96:PHE:O	1:D:100:LEU:HD22	2.10	0.51
1:B:339:LYS:HA	1:B:367:HIS:CE1	2.46	0.51
1:B:69:HIS:HE1	1:B:102:ASP:OD2	1.93	0.51
1:B:41:THR:OG1	1:B:44:GLU:HG3	2.10	0.51
1:D:177:MSE:HE2	1:D:181:VAL:CG2	2.30	0.51
1:D:339:LYS:HE3	6:D:2100:HOH:O	2.10	0.51
1:A:478:VAL:HG13	1:A:483:THR:HB	1.92	0.51
1:C:307:ILE:N	1:C:307:ILE:HD12	2.25	0.51
1:B:421:ASN:ND2	3:B:603:TTN:O4	2.43	0.51
1:D:140:ARG:HH22	1:D:233:ASP:CB	2.16	0.51
1:B:150:TRP:CE2	1:B:199:LEU:HD13	2.45	0.51
1:D:107:LEU:O	1:D:111:VAL:HG12	2.11	0.51
1:A:232:ASP:CG	1:A:264:ARG:HH22	2.14	0.51
1:D:261:ASN:HD22	1:D:264:ARG:HE	1.59	0.51
1:B:165:ARG:NH1	2:B:601:ATP:O2B	2.43	0.51
1:C:260:HIS:CD2	1:C:264:ARG:HH21	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ALA:O	1:C:291:LEU:HD22	2.10	0.51
1:B:184:LEU:HD22	1:B:198:CYS:HB3	1.93	0.51
1:D:51:GLN:HA	1:D:51:GLN:HE21	1.76	0.51
1:C:308:LEU:HB3	1:C:389:ILE:HD12	1.94	0.50
1:A:286:VAL:HG22	1:A:470:ILE:CG1	2.41	0.50
1:C:380:ALA:O	1:C:384:LEU:HD13	2.11	0.50
1:B:243:THR:HG21	1:B:273:TYR:CD2	2.47	0.50
1:A:506:GLU:HA	1:A:509:GLN:NE2	2.27	0.50
1:D:308:LEU:HB3	1:D:389:ILE:CD1	2.39	0.50
1:D:175:TYR:HE2	1:D:219:MSE:HG2	1.77	0.50
1:D:85:ILE:HG13	1:D:86:MSE:N	2.27	0.50
1:A:471:PHE:CG	1:A:472:PRO:HD3	2.47	0.50
1:C:108:MSE:HB3	1:C:109:PRO:HD3	1.93	0.50
1:B:286:VAL:HG22	1:B:470:ILE:CG1	2.42	0.50
1:D:243:THR:HG21	1:D:273:TYR:CD2	2.47	0.50
1:B:43:GLN:HG2	1:B:47:MSE:CE	2.32	0.49
1:C:300:LYS:HZ2	1:C:300:LYS:HB3	1.77	0.49
1:B:332:LEU:CD1	1:B:332:LEU:H	2.25	0.49
1:D:453:LYS:HZ1	1:D:457:GLY:HA2	1.75	0.49
1:C:41:THR:O	1:C:45:ARG:HG3	2.12	0.49
1:B:350:LEU:HD22	1:B:354:ARG:NH2	2.26	0.49
1:B:232:ASP:OD1	1:B:264:ARG:NH2	2.44	0.49
1:B:302:ILE:HD12	1:B:305:HIS:ND1	2.26	0.49
1:D:478:VAL:HG13	1:D:483:THR:HB	1.93	0.49
1:D:284:ALA:HA	1:D:319:ILE:HG12	1.95	0.49
1:A:328:VAL:HA	1:A:332:LEU:O	2.13	0.49
1:B:492:LEU:CD2	1:B:496:LYS:HE3	2.37	0.49
1:A:389:ILE:HG23	1:A:399:PHE:CZ	2.47	0.49
1:A:466:ASN:ND2	3:A:603:TTN:O4	2.45	0.49
1:C:502:LEU:HD23	1:C:503:THR:O	2.12	0.49
1:C:40:PHE:HE2	1:C:565:LEU:HD12	1.76	0.49
1:A:65:ALA:HA	1:A:99:ILE:HD11	1.94	0.49
1:C:282:GLY:O	1:C:286:VAL:HG23	2.13	0.48
1:C:315:ALA:HB3	1:C:392:VAL:CG2	2.42	0.48
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.94	0.48
1:D:528:ILE:HA	1:D:531:THR:CG2	2.44	0.48
1:C:184:LEU:O	1:C:187:TYR:HB2	2.13	0.48
1:D:476:LEU:O	1:D:480:LEU:HG	2.13	0.48
1:C:312:ALA:HB1	1:C:343:MSE:CE	2.43	0.48
1:C:392:VAL:CG1	1:C:392:VAL:O	2.58	0.48
1:B:502:LEU:HD11	1:B:512:LEU:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:O	1:B:46:GLN:HG3	2.13	0.48
1:A:544:PRO:HD3	1:D:248:ARG:HH12	1.77	0.48
1:C:478:VAL:HG13	1:C:483:THR:HB	1.96	0.48
1:C:302:ILE:CD1	1:C:332:LEU:HD13	2.44	0.48
1:D:520:GLN:O	1:D:524:ILE:HG12	2.14	0.48
1:B:85:ILE:HD12	1:B:86:MSE:N	2.29	0.48
1:C:391:GLY:HA3	1:C:427:GLU:HG2	1.96	0.48
1:B:75:MSE:HE1	1:B:84:TYR:CD2	2.48	0.48
1:C:338:GLN:NE2	1:C:364:PRO:CB	2.75	0.47
1:D:503:THR:OG1	1:D:506:GLU:HG3	2.13	0.47
1:A:339:LYS:NZ	1:A:339:LYS:HB2	2.28	0.47
1:D:194:ARG:NH1	1:D:194:ARG:HG2	2.28	0.47
1:C:319:ILE:O	1:C:323:ILE:HG13	2.15	0.47
1:A:395:ALA:HB1	6:A:2097:HOH:O	2.13	0.47
1:D:319:ILE:O	1:D:323:ILE:HG13	2.15	0.47
1:A:384:LEU:N	1:A:384:LEU:CD1	2.77	0.47
1:A:333:SER:H	1:A:336:GLU:CG	2.26	0.47
1:C:432:GLU:O	1:C:436:LEU:HB2	2.14	0.47
1:B:81:LYS:O	1:B:85:ILE:HG23	2.13	0.47
1:B:484:ARG:HG2	1:C:543:TYR:CZ	2.49	0.47
1:C:286:VAL:HG22	1:C:470:ILE:CG1	2.44	0.47
1:A:389:ILE:HG23	1:A:399:PHE:CE1	2.49	0.47
1:A:40:PHE:HE2	1:A:565:LEU:HD12	1.80	0.47
1:B:556:ARG:HG3	1:B:556:ARG:NH1	2.29	0.47
1:D:143:VAL:HB	1:D:237:GLU:HG2	1.96	0.47
1:D:492:LEU:HD22	1:D:496:LYS:HE2	1.96	0.47
1:D:156:LYS:HE3	6:D:2079:HOH:O	2.15	0.47
1:A:130:PRO:HG3	1:B:54:LEU:HD23	1.96	0.47
1:B:312:ALA:HB1	1:B:343:MSE:HE3	1.98	0.47
1:C:137:ILE:HA	1:C:234:LEU:HD22	1.97	0.47
1:C:384:LEU:N	1:C:384:LEU:CD1	2.78	0.46
1:B:502:LEU:HD13	1:B:507:LEU:CD2	2.45	0.46
1:C:556:ARG:HG3	1:C:556:ARG:HH11	1.80	0.46
1:A:407:MSE:CE	1:A:407:MSE:HA	2.39	0.46
1:A:288:LEU:O	1:A:292:LEU:HD23	2.16	0.46
1:D:187:TYR:CD2	1:D:193:ILE:HD12	2.50	0.46
1:B:369:ALA:HB1	1:B:373:ILE:CD1	2.36	0.46
1:D:332:LEU:N	1:D:332:LEU:HD12	2.27	0.46
1:C:389:ILE:HG23	1:C:399:PHE:CE1	2.50	0.46
1:D:82:TYR:CE1	1:D:86:MSE:HE3	2.51	0.46
1:C:261:ASN:ND2	1:C:264:ARG:NH2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:GLN:NE2	1:D:562:TYR:OH	2.44	0.46
1:A:325:MSE:HA	1:A:328:VAL:HG22	1.96	0.46
1:D:239:MSE:HE1	1:D:254:PHE:CZ	2.47	0.46
1:B:389:ILE:HG22	1:B:416:ILE:HA	1.97	0.46
1:C:280:ILE:O	1:C:284:ALA:HB2	2.14	0.46
1:B:520:GLN:HE21	1:B:520:GLN:N	2.04	0.46
1:D:535:TYR:CD2	1:D:545:GLU:HG3	2.50	0.46
1:A:550:ALA:O	1:A:554:LYS:HG3	2.15	0.46
1:C:261:ASN:ND2	1:C:264:ARG:HH22	2.13	0.46
1:A:146:ILE:HG23	1:B:52:GLY:HA3	1.98	0.46
1:B:502:LEU:HD13	1:B:507:LEU:HD21	1.98	0.46
1:B:332:LEU:N	1:B:332:LEU:HD12	2.31	0.46
1:A:214:LYS:HG3	6:A:2062:HOH:O	2.15	0.46
1:B:354:ARG:NE	1:B:358:ILE:HD11	2.31	0.46
1:C:328:VAL:HA	1:C:332:LEU:O	2.15	0.46
1:B:332:LEU:N	1:B:332:LEU:CD1	2.80	0.46
1:A:166:ILE:HG23	1:A:179:ILE:HG13	1.97	0.45
1:D:300:LYS:HB3	1:D:300:LYS:HZ2	1.81	0.45
1:D:502:LEU:HD13	1:D:507:LEU:HD21	1.98	0.45
1:A:154:HIS:HD2	6:A:2073:HOH:O	1.98	0.45
1:C:559:ARG:HB3	1:C:561:GLU:HG2	1.99	0.45
1:C:73:LYS:HA	1:C:73:LYS:CE	2.42	0.45
1:B:312:ALA:HB1	1:B:343:MSE:CE	2.46	0.45
1:B:213:LEU:HD11	1:B:224:LYS:HD3	1.99	0.45
1:D:122:GLN:HE21	1:D:122:GLN:HB3	1.52	0.45
1:C:308:LEU:HD12	1:C:309:PHE:N	2.32	0.45
1:B:307:ILE:HD13	1:B:323:ILE:HD13	1.99	0.45
1:A:282:GLY:O	1:A:286:VAL:HG23	2.17	0.45
1:D:551:LYS:CB	1:D:551:LYS:HZ2	2.30	0.45
1:D:165:ARG:NH2	3:D:603:TTN:O1	2.47	0.45
1:B:518:ASN:HB3	1:B:521:GLU:CD	2.37	0.44
1:C:315:ALA:HB1	1:C:392:VAL:HG21	1.99	0.44
1:A:546:PRO:O	1:A:549:LYS:HE2	2.17	0.44
1:C:349:LEU:HD22	1:C:374:PRO:HG3	1.99	0.44
1:D:188:THR:HG21	1:D:195:PRO:HG3	1.99	0.44
1:D:239:MSE:CE	1:D:254:PHE:HZ	2.28	0.44
1:D:412:GLU:O	1:D:413:ARG:HD2	2.17	0.44
1:A:46:GLN:HG2	1:A:51:GLN:HG3	2.00	0.44
1:D:556:ARG:HH11	1:D:556:ARG:HG3	1.83	0.44
1:C:320:ALA:O	1:C:324:VAL:HG23	2.16	0.44
1:A:552:TYR:CE1	1:A:556:ARG:CZ	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:LEU:HD12	1:D:322:LEU:HA	1.82	0.44
1:B:284:ALA:HA	1:B:319:ILE:HG12	1.99	0.44
1:B:308:LEU:HB3	1:B:389:ILE:CD1	2.47	0.44
1:C:210:ILE:O	1:C:214:LYS:HG3	2.17	0.44
1:D:183:LYS:HE3	1:D:255:GLU:OE2	2.17	0.44
1:C:166:ILE:HD12	1:C:179:ILE:HG13	1.99	0.44
1:D:172:LEU:O	1:D:175:TYR:HB2	2.16	0.44
1:D:506:GLU:OE2	1:D:515:PRO:HD3	2.18	0.44
1:D:158:VAL:HG22	1:D:199:LEU:HB3	2.00	0.44
1:A:520:GLN:HB2	6:A:2126:HOH:O	2.16	0.44
1:A:33:ARG:NH1	1:A:93:GLU:OE1	2.49	0.44
1:A:325:MSE:O	1:A:328:VAL:HG22	2.17	0.44
1:A:120:CYS:O	1:A:175:TYR:HB3	2.17	0.44
1:C:218:TYR:O	1:D:57:LYS:HD3	2.17	0.44
1:B:29:MSE:HE1	1:B:53:LEU:HD13	1.98	0.44
1:B:110:ILE:HD12	1:B:110:ILE:N	2.33	0.44
1:C:377:PHE:CZ	1:C:389:ILE:HD11	2.53	0.44
1:A:204:ASP:OD2	1:B:56:PRO:HG2	2.18	0.44
1:B:329:GLU:HG2	1:B:329:GLU:O	2.18	0.44
1:B:77:SER:HB2	6:B:2015:HOH:O	2.18	0.44
1:B:515:PRO:CG	1:B:518:ASN:HD22	2.21	0.44
1:B:261:ASN:ND2	1:B:264:ARG:HH11	2.15	0.44
1:B:333:SER:H	1:B:336:GLU:CG	2.30	0.44
1:A:308:LEU:HD23	1:A:389:ILE:HD11	2.00	0.44
1:C:484:ARG:NH2	1:C:541:PHE:CD2	2.85	0.44
1:C:81:LYS:O	1:C:85:ILE:HG23	2.18	0.43
1:B:297:VAL:CG2	1:B:442:LEU:HD11	2.47	0.43
1:B:317:LEU:HD13	1:B:361:TYR:HB3	2.00	0.43
1:B:327:MSE:CE	1:B:337:ALA:HB1	2.48	0.43
1:D:194:ARG:HA	1:D:195:PRO:HD3	1.91	0.43
1:D:492:LEU:HD23	1:D:492:LEU:O	2.19	0.43
1:D:78:PRO:HD2	6:D:2014:HOH:O	2.17	0.43
1:A:387:SER:HA	1:A:411:ASN:OD1	2.19	0.43
1:B:528:ILE:HD13	1:B:550:ALA:HA	1.99	0.43
1:C:363:GLU:HB3	1:C:364:PRO:HD3	2.00	0.43
1:D:150:TRP:HA	1:D:151:PRO:HD3	1.78	0.43
1:B:85:ILE:CD1	1:B:86:MSE:SE	3.14	0.43
1:A:91:ARG:HH21	5:A:605:FUM:C2	2.30	0.43
1:B:45:ARG:HB2	1:B:51:GLN:HE21	1.83	0.43
1:B:294:ALA:O	1:B:297:VAL:HG22	2.18	0.43
1:A:341:ILE:O	1:A:367:HIS:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:O	1:B:175:TYR:HB2	2.19	0.43
1:C:184:LEU:HD12	1:C:200:PRO:CG	2.41	0.43
1:C:85:ILE:HD12	1:C:86:MSE:N	2.34	0.43
1:A:288:LEU:HG	1:A:292:LEU:CD2	2.49	0.43
1:C:240:LYS:HD2	6:C:2071:HOH:O	2.19	0.43
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.99	0.43
1:C:284:ALA:HA	1:C:319:ILE:HG12	2.01	0.43
1:C:111:VAL:HG22	1:C:111:VAL:O	2.19	0.43
1:C:75:MSE:HE1	1:C:84:TYR:CG	2.53	0.43
1:B:291:LEU:HD13	1:B:417:PHE:CE2	2.53	0.43
1:B:66:LEU:HD22	1:B:70:ARG:HH11	1.78	0.42
1:C:169:LEU:HD13	1:C:422:PRO:HD2	2.01	0.42
1:B:66:LEU:HD13	1:B:70:ARG:HH12	1.84	0.42
1:B:354:ARG:HE	1:B:358:ILE:HD11	1.84	0.42
1:D:261:ASN:ND2	1:D:264:ARG:HH21	2.17	0.42
1:A:26:LYS:HB3	1:A:27:PRO:HD3	2.00	0.42
1:B:289:ALA:CB	1:B:498:LEU:HD23	2.49	0.42
1:A:432:GLU:O	1:A:436:LEU:HD13	2.20	0.42
1:C:369:ALA:HB1	1:C:373:ILE:CD1	2.46	0.42
1:D:41:THR:OG1	1:D:44:GLU:HG3	2.19	0.42
1:A:324:VAL:O	1:A:328:VAL:HG13	2.20	0.42
1:C:69:HIS:HE1	1:C:102:ASP:OD2	2.02	0.42
1:C:146:ILE:HG23	1:D:52:GLY:HA3	2.02	0.42
1:B:85:ILE:CD1	1:B:111:VAL:HG22	2.48	0.42
1:B:132:GLY:HA2	1:B:200:PRO:HG2	2.02	0.42
1:B:380:ALA:O	1:B:384:LEU:HD23	2.20	0.42
1:D:394:GLY:HA2	1:D:420:SER:HB3	2.01	0.42
1:C:186:LEU:HD13	1:C:468:VAL:HG23	2.02	0.42
1:B:520:GLN:O	1:B:524:ILE:HG12	2.19	0.42
1:A:401:PRO:HA	1:A:436:LEU:CD2	2.50	0.42
1:B:487:SER:OG	1:B:539:MSE:HE1	2.19	0.42
1:B:532:GLU:HG2	1:B:549:LYS:HG2	2.01	0.42
1:A:273:TYR:HB3	6:A:2074:HOH:O	2.20	0.42
1:A:308:LEU:HB3	1:A:389:ILE:HD12	2.01	0.42
1:C:38:MSE:HE3	1:C:59:GLU:OE1	2.19	0.42
1:B:505:GLU:H	1:B:505:GLU:CD	2.23	0.42
1:C:261:ASN:HD22	1:C:264:ARG:NH2	2.17	0.42
1:A:108:MSE:N	1:A:109:PRO:CD	2.82	0.42
1:B:263:PHE:CZ	1:B:314:GLU:HA	2.55	0.42
1:A:566:LEU:HA	1:A:567:PRO:HD3	1.95	0.42
1:D:324:VAL:O	1:D:328:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:HG	1:B:99:ILE:HD12	2.01	0.42
1:B:328:VAL:HA	1:B:332:LEU:O	2.20	0.42
1:D:542:ARG:HH12	1:D:544:PRO:HD2	1.85	0.42
1:A:90:GLU:OE1	1:A:131:LYS:HE2	2.20	0.42
1:A:104:ILE:HG13	1:A:108:MSE:HE2	2.02	0.41
1:B:493:GLU:HG3	1:B:533:TYR:CE1	2.55	0.41
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.34	0.41
1:D:140:ARG:NH2	1:D:230:GLN:O	2.54	0.41
1:A:86:MSE:SE	1:A:111:VAL:HG23	2.71	0.41
1:D:389:ILE:HG23	1:D:399:PHE:CE1	2.55	0.41
1:A:45:ARG:HA	1:A:50:LEU:HB2	2.02	0.41
1:C:70:ARG:O	1:C:74:LYS:HD3	2.20	0.41
1:C:154:HIS:O	1:C:197:ARG:HD2	2.20	0.41
1:B:253:GLN:NE2	1:B:255:GLU:OE2	2.51	0.41
1:C:350:LEU:HD12	1:C:358:ILE:HD12	2.01	0.41
1:A:68:PHE:CD2	1:A:99:ILE:HG13	2.55	0.41
1:A:188:THR:HG21	1:A:195:PRO:HG3	2.01	0.41
1:A:194:ARG:HA	1:A:195:PRO:HD3	1.91	0.41
1:C:466:ASN:ND2	3:C:603:TTN:O4	2.52	0.41
1:C:271:GLU:OE2	1:C:271:GLU:HA	2.19	0.41
1:D:328:VAL:HA	1:D:332:LEU:O	2.21	0.41
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.68	0.41
1:D:502:LEU:HD11	1:D:512:LEU:C	2.41	0.41
1:B:75:MSE:HE1	1:B:84:TYR:CG	2.56	0.41
1:B:454:LEU:CD1	1:B:460:PHE:HE2	2.33	0.41
1:A:383:ILE:HG22	1:A:384:LEU:HD12	2.01	0.41
1:B:108:MSE:N	1:B:109:PRO:CD	2.84	0.41
1:D:506:GLU:O	1:D:511:ARG:HB2	2.20	0.41
1:C:165:ARG:NH1	2:C:601:ATP:O2B	2.52	0.41
1:B:542:ARG:HD3	1:B:543:TYR:N	2.36	0.41
1:C:369:ALA:CB	1:C:373:ILE:HD11	2.47	0.41
1:C:264:ARG:HG2	1:C:264:ARG:HH11	1.86	0.41
1:B:177:MSE:O	1:B:180:PRO:HD2	2.21	0.41
1:C:442:LEU:HD23	1:C:442:LEU:HA	1.95	0.41
1:D:109:PRO:HA	1:D:113:THR:O	2.21	0.41
1:C:389:ILE:HG22	1:C:416:ILE:HA	2.03	0.41
1:B:401:PRO:O	1:B:405:ARG:HG3	2.21	0.41
1:D:294:ALA:O	1:D:297:VAL:HG22	2.21	0.41
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.57	0.41
1:A:242:ILE:HA	1:A:242:ILE:HD13	1.95	0.41
1:A:52:GLY:HA3	1:B:146:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASN:HB2	1:A:414:PRO:HB3	2.03	0.40
1:D:363:GLU:HB2	1:D:364:PRO:HD3	2.02	0.40
1:B:233:ASP:CG	1:B:234:LEU:N	2.75	0.40
1:A:243:THR:HG21	1:A:273:TYR:HD2	1.86	0.40
1:C:412:GLU:O	1:C:413:ARG:HD2	2.22	0.40
1:C:150:TRP:HA	1:C:151:PRO:HD3	1.86	0.40
1:B:40:PHE:HE2	1:B:565:LEU:HD12	1.86	0.40
1:A:298:ILE:HD11	1:A:442:LEU:HD12	2.04	0.40
1:C:61:GLN:HA	1:C:64:GLN:HE21	1.86	0.40
1:D:33:ARG:HH21	1:D:152:GLU:HG3	1.87	0.40
1:C:154:HIS:O	1:C:197:ARG:CD	2.70	0.40
1:B:120:CYS:O	1:B:175:TYR:HB3	2.22	0.40
1:C:97:TYR:CE2	1:C:188:THR:HB	2.56	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	549/551 (100%)	531 (97%)	17 (3%)	1 (0%)	52	59
1	B	549/551 (100%)	530 (96%)	17 (3%)	2 (0%)	39	42
1	C	549/551 (100%)	528 (96%)	20 (4%)	1 (0%)	52	59
1	D	549/551 (100%)	527 (96%)	21 (4%)	1 (0%)	52	59
All	All	2196/2204 (100%)	2116 (96%)	75 (3%)	5 (0%)	52	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	ARG
1	B	397	ARG

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Mol	Chain	Res	Type
1	D	397	ARG
1	C	392	VAL
1	B	392	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	467/453 (103%)	445 (95%)	22 (5%)	32	39
1	B	467/453 (103%)	448 (96%)	19 (4%)	37	45
1	C	467/453 (103%)	445 (95%)	22 (5%)	32	39
1	D	467/453 (103%)	438 (94%)	29 (6%)	23	25
All	All	1868/1812 (103%)	1776 (95%)	92 (5%)	31	36

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	PRO
1	A	70	ARG
1	A	85	ILE
1	A	99	ILE
1	A	100	LEU
1	A	123	TYR
1	A	152	GLU
1	A	169	LEU
1	A	221	LEU
1	A	225	ARG
1	A	248	ARG
1	A	251	LEU
1	A	291	LEU
1	A	339	LYS
1	A	350	LEU
1	A	492	LEU
1	A	502	LEU
1	A	505	GLU

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Mol	Chain	Res	Type
1	A	506	GLU
1	A	520	GLN
1	A	559	ARG
1	A	561	GLU
1	B	99	ILE
1	B	100	LEU
1	B	123	TYR
1	B	133	LEU
1	B	165	ARG
1	B	169	LEU
1	B	221	LEU
1	B	233	ASP
1	B	251	LEU
1	B	291	LEU
1	B	350	LEU
1	B	371	GLU
1	B	398	LEU
1	B	436	LEU
1	B	492	LEU
1	B	504	ASP
1	B	520	GLN
1	B	559	ARG
1	B	572	TRP
1	C	66	LEU
1	C	70	ARG
1	C	73	LYS
1	C	114	PRO
1	C	123	TYR
1	C	133	LEU
1	C	165	ARG
1	C	169	LEU
1	C	242	ILE
1	C	251	LEU
1	C	300	LYS
1	C	306	LYS
1	C	339	LYS
1	C	359	ASP
1	C	371	GLU
1	C	436	LEU
1	C	455	THR
1	C	507	LEU
1	C	520	GLN

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Mol	Chain	Res	Type
1	C	547	GLU
1	C	559	ARG
1	C	561	GLU
1	D	33	ARG
1	D	51	GLN
1	D	74	LYS
1	D	85	ILE
1	D	99	ILE
1	D	100	LEU
1	D	122	GLN
1	D	123	TYR
1	D	133	LEU
1	D	140	ARG
1	D	153	ASN
1	D	165	ARG
1	D	169	LEU
1	D	219	MSE
1	D	221	LEU
1	D	229	GLN
1	D	251	LEU
1	D	266	LEU
1	D	291	LEU
1	D	292	LEU
1	D	300	LYS
1	D	363	GLU
1	D	371	GLU
1	D	409	SER
1	D	425	GLN
1	D	520	GLN
1	D	531	THR
1	D	547	GLU
1	D	561	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	64	GLN
1	A	154	HIS
1	A	230	GLN
1	A	261	ASN
1	A	330	ASN

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Mol	Chain	Res	Type
1	A	425	GLN
1	A	482	ASN
1	A	485	HIS
1	A	520	GLN
1	B	43	GLN
1	B	51	GLN
1	B	64	GLN
1	B	69	HIS
1	B	154	HIS
1	B	229	GLN
1	B	230	GLN
1	B	261	ASN
1	B	335	GLN
1	B	482	ASN
1	B	518	ASN
1	B	520	GLN
1	C	64	GLN
1	C	69	HIS
1	C	154	HIS
1	C	229	GLN
1	C	230	GLN
1	C	261	ASN
1	C	305	HIS
1	C	338	GLN
1	C	520	GLN
1	D	43	GLN
1	D	51	GLN
1	D	64	GLN
1	D	69	HIS
1	D	89	GLN
1	D	122	GLN
1	D	125	HIS
1	D	230	GLN
1	D	261	ASN
1	D	425	GLN
1	D	482	ASN
1	D	520	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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$
2	ATP	A	601	-	24,33,33	1.56	5 (20%)	31,52,52	2.33	3 (9%)
2	ATP	A	602	-	24,33,33	1.70	5 (20%)	31,52,52	2.28	2 (6%)
3	TTN	A	603	4	1,7,7	0.06	0	2,9,9	0.82	0
5	FUM	A	605	-	1,7,7	1.67	0	0,8,8	0.00	-
2	ATP	B	601	-	24,33,33	1.62	4 (16%)	31,52,52	2.30	3 (9%)
2	ATP	B	602	-	24,33,33	1.59	5 (20%)	31,52,52	2.28	2 (6%)
3	TTN	B	603	4	1,7,7	0.13	0	2,9,9	1.00	0
5	FUM	B	605	-	1,7,7	1.69	0	0,8,8	0.00	-
2	ATP	C	601	-	24,33,33	1.59	5 (20%)	31,52,52	2.34	4 (12%)
2	ATP	C	602	-	24,33,33	1.64	5 (20%)	31,52,52	2.22	2 (6%)
3	TTN	C	603	4	1,7,7	0.22	0	2,9,9	0.60	0
5	FUM	C	605	-	1,7,7	1.99	0	0,8,8	0.00	-
2	ATP	D	601	-	24,33,33	1.61	5 (20%)	31,52,52	2.32	4 (12%)
2	ATP	D	602	-	24,33,33	1.62	5 (20%)	31,52,52	2.26	2 (6%)
3	TTN	D	603	4	1,7,7	0.18	0	2,9,9	1.09	0
5	FUM	D	605	-	1,7,7	1.69	0	0,8,8	0.00	-

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
2	ATP	A	601	-	-	0/18/38/38	0/3/3/3
2	ATP	A	602	-	-	0/18/38/38	0/3/3/3
3	TTN	A	603	4	-	0/0/8/8	0/0/0/0
5	FUM	A	605	-	-	0/0/5/5	0/0/0/0
2	ATP	B	601	-	-	0/18/38/38	0/3/3/3
2	ATP	B	602	-	-	0/18/38/38	0/3/3/3
3	TTN	B	603	4	-	0/0/8/8	0/0/0/0
5	FUM	B	605	-	-	0/0/5/5	0/0/0/0
2	ATP	C	601	-	-	0/18/38/38	0/3/3/3
2	ATP	C	602	-	-	0/18/38/38	0/3/3/3
3	TTN	C	603	4	-	0/0/8/8	0/0/0/0
5	FUM	C	605	-	-	0/0/5/5	0/0/0/0
2	ATP	D	601	-	-	0/18/38/38	0/3/3/3
2	ATP	D	602	-	-	0/18/38/38	0/3/3/3
3	TTN	D	603	4	-	0/0/8/8	0/0/0/0
5	FUM	D	605	-	-	0/0/5/5	0/0/0/0

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ATP	C5-C4	-3.19	1.33	1.40
2	C	602	ATP	C5-C4	-3.16	1.33	1.40
2	C	601	ATP	C5-C4	-3.11	1.33	1.40
2	D	601	ATP	C5-C4	-3.09	1.33	1.40
2	A	602	ATP	C5-C4	-2.92	1.33	1.40
2	A	601	ATP	C5-C4	-2.89	1.34	1.40
2	B	602	ATP	C5-C4	-2.72	1.34	1.40
2	D	602	ATP	C5-C4	-2.68	1.34	1.40
2	D	602	ATP	C5-N7	-2.52	1.30	1.39
2	B	601	ATP	C5-N7	-2.47	1.31	1.39
2	A	602	ATP	C5-N7	-2.44	1.31	1.39
2	C	602	ATP	C5-N7	-2.44	1.31	1.39
2	D	601	ATP	C5-N7	-2.41	1.31	1.39
2	C	601	ATP	C5-N7	-2.39	1.31	1.39
2	A	601	ATP	C5-N7	-2.35	1.31	1.39
2	B	602	ATP	C5-N7	-2.33	1.31	1.39
2	C	601	ATP	C2-N1	2.02	1.37	1.33
2	D	601	ATP	C2-N1	2.06	1.37	1.33
2	B	602	ATP	C2-N1	2.14	1.38	1.33
2	C	602	ATP	C2-N1	2.16	1.38	1.33
2	A	602	ATP	C2-N1	2.17	1.38	1.33
2	A	601	ATP	C2-N1	2.27	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	ATP	C2-N1	2.44	1.38	1.33
2	B	601	ATP	C2-N3	2.78	1.37	1.32
2	D	601	ATP	C2-N3	2.82	1.37	1.32
2	C	602	ATP	C2-N3	2.84	1.37	1.32
2	C	601	ATP	C2-N3	2.87	1.37	1.32
2	A	602	ATP	C2-N3	2.88	1.37	1.32
2	B	602	ATP	C2-N3	2.96	1.37	1.32
2	D	602	ATP	C2-N3	3.00	1.37	1.32
2	A	601	ATP	C2-N3	3.04	1.37	1.32
2	A	601	ATP	O4'-C1'	3.46	1.45	1.41
2	B	602	ATP	O4'-C1'	3.72	1.45	1.41
2	C	601	ATP	O4'-C1'	3.72	1.45	1.41
2	D	602	ATP	O4'-C1'	3.89	1.46	1.41
2	C	602	ATP	O4'-C1'	4.16	1.46	1.41
2	B	601	ATP	O4'-C1'	4.19	1.46	1.41
2	D	601	ATP	O4'-C1'	4.40	1.46	1.41
2	A	602	ATP	O4'-C1'	4.71	1.47	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	ATP	N3-C2-N1	-10.86	120.58	128.89
2	A	601	ATP	N3-C2-N1	-10.83	120.60	128.89
2	A	602	ATP	N3-C2-N1	-10.82	120.61	128.89
2	B	602	ATP	N3-C2-N1	-10.82	120.61	128.89
2	D	601	ATP	N3-C2-N1	-10.79	120.64	128.89
2	B	601	ATP	N3-C2-N1	-10.66	120.73	128.89
2	D	602	ATP	N3-C2-N1	-10.58	120.79	128.89
2	C	602	ATP	N3-C2-N1	-10.47	120.88	128.89
2	C	601	ATP	C4'-O4'-C1'	-2.34	107.15	109.72
2	D	601	ATP	C4'-O4'-C1'	-2.26	107.23	109.72
2	A	601	ATP	C4'-O4'-C1'	-2.07	107.45	109.72
2	C	601	ATP	O4'-C1'-N9	2.19	112.69	108.10
2	B	601	ATP	O4'-C1'-N9	2.21	112.72	108.10
2	D	601	ATP	O4'-C1'-N9	2.28	112.86	108.10
2	C	602	ATP	C4-C5-N7	4.50	113.62	109.48
2	B	602	ATP	C4-C5-N7	4.60	113.71	109.48
2	D	601	ATP	C4-C5-N7	4.62	113.73	109.48
2	C	601	ATP	C4-C5-N7	4.62	113.73	109.48
2	B	601	ATP	C4-C5-N7	4.64	113.75	109.48
2	A	602	ATP	C4-C5-N7	4.70	113.81	109.48
2	A	601	ATP	C4-C5-N7	4.79	113.88	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	602	ATP	C4-C5-N7	4.80	113.89	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	TTN	1	0
5	A	605	FUM	1	0
2	B	601	ATP	1	0
3	B	603	TTN	1	0
2	C	601	ATP	1	0
3	C	603	TTN	1	0
3	D	603	TTN	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.