



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:51 am GMT

PDB ID : 4BUB
Title : CRYSTAL STRUCTURE OF MURE LIGASE FROM THERMOTOGA MARITIMA IN COMPLEX WITH ADP
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Deposited on : 2013-06-20
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

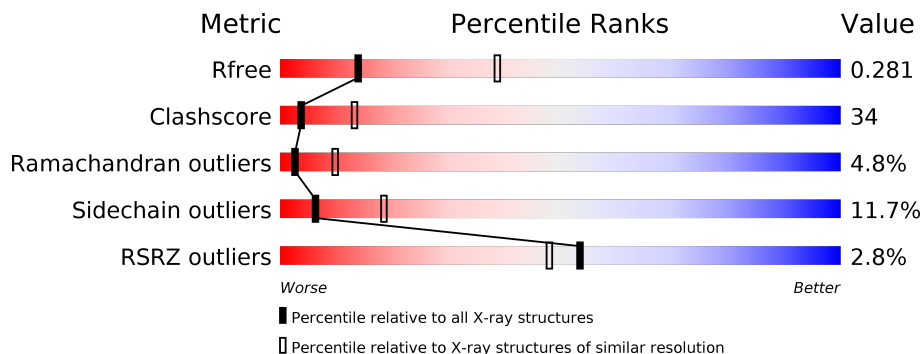
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	498	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>41%</div> <div>7%</div> <div></div> </div> </div>
1	B	498	<div> <div>3%</div> <div> <div></div> <div>41%</div> <div>47%</div> <div>9%</div> <div></div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7620 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.

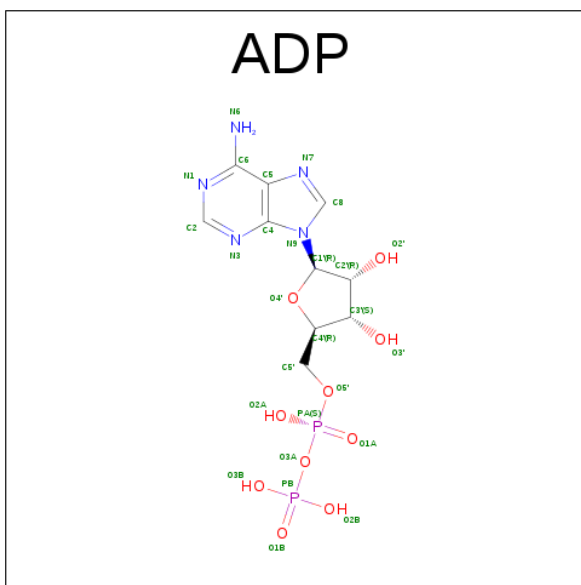
- Molecule 1 is a protein called UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--LD-LYSINE LIGASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	Se	0	0	0
			3755	2382	648	715	1	9			
1	B	483	Total	C	N	O	S	Se	0	0	0
			3792	2402	655	725	1	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	491	LEU	-	EXPRESSION TAG	UNP Q9WY79
A	492	GLU	-	EXPRESSION TAG	UNP Q9WY79
A	493	HIS	-	EXPRESSION TAG	UNP Q9WY79
A	494	HIS	-	EXPRESSION TAG	UNP Q9WY79
A	495	HIS	-	EXPRESSION TAG	UNP Q9WY79
A	496	HIS	-	EXPRESSION TAG	UNP Q9WY79
A	497	HIS	-	EXPRESSION TAG	UNP Q9WY79
A	498	HIS	-	EXPRESSION TAG	UNP Q9WY79
B	491	LEU	-	EXPRESSION TAG	UNP Q9WY79
B	492	GLU	-	EXPRESSION TAG	UNP Q9WY79
B	493	HIS	-	EXPRESSION TAG	UNP Q9WY79
B	494	HIS	-	EXPRESSION TAG	UNP Q9WY79
B	495	HIS	-	EXPRESSION TAG	UNP Q9WY79
B	496	HIS	-	EXPRESSION TAG	UNP Q9WY79
B	497	HIS	-	EXPRESSION TAG	UNP Q9WY79
B	498	HIS	-	EXPRESSION TAG	UNP Q9WY79

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

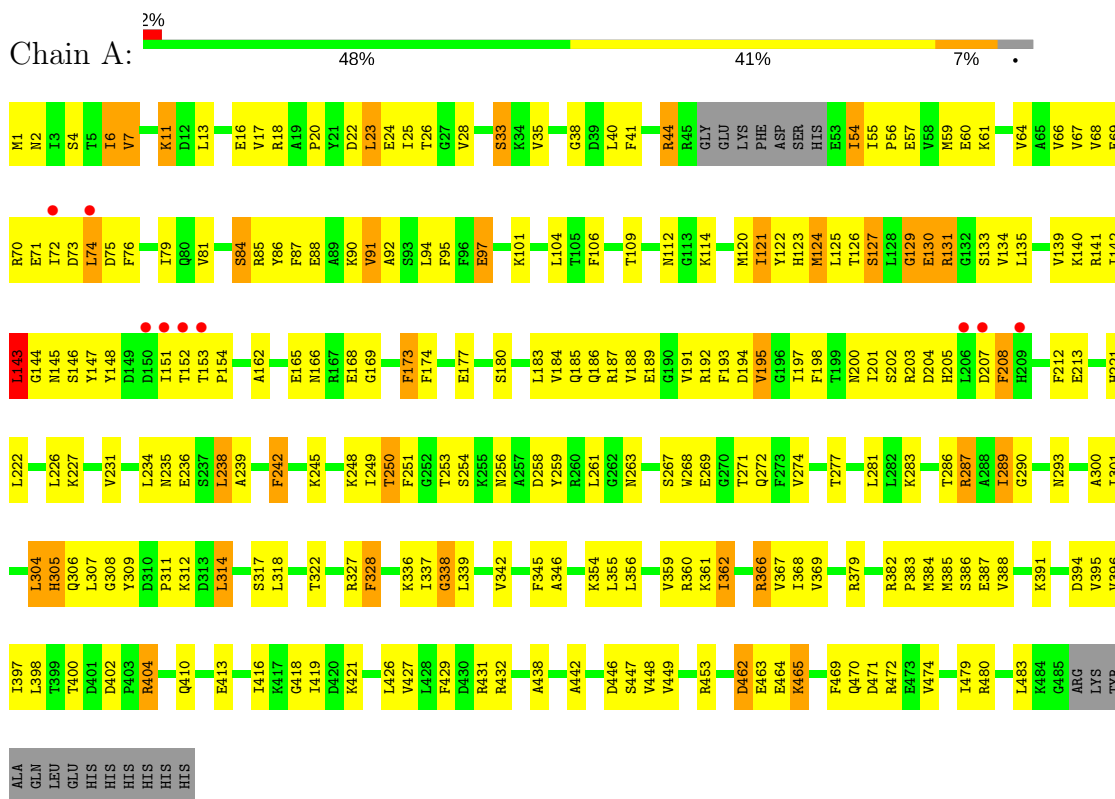
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	B	7	Total O 7 7	0	0

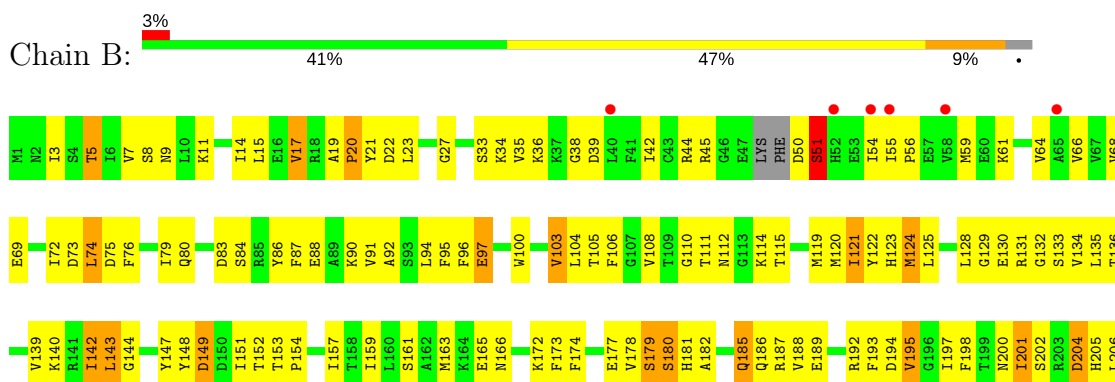
3 Residue-property plots [i](#)

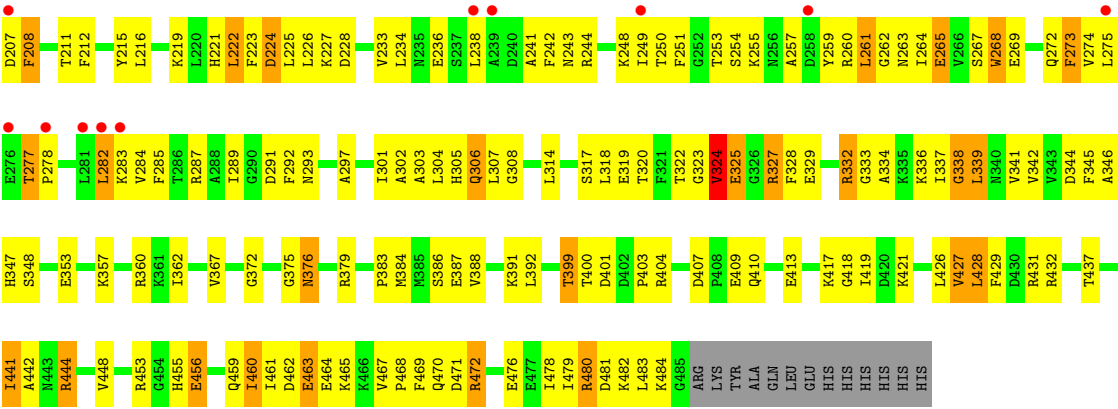
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--LD-LYSINE LIGASE



• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--LD-LYSINE LIGASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	74.39Å 74.39Å 441.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.48 – 2.90 48.48 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.48-2.90) 96.0 (48.48-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.218 , 0.281 0.214 , 0.281	Depositor DCC
R_{free} test set	2909 reflections (11.05%)	DCC
Wilson B-factor (Å ²)	91.7	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.109 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7620	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, 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	0.45	0/3808	0.62	0/5124
1	B	0.44	0/3846	0.60	0/5175
All	All	0.45	0/7654	0.61	0/10299

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	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	204	ASP	Peptide
1	B	338	GLY	Peptide

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	3755	0	3790	233	1
1	B	3792	0	3815	290	1
2	A	27	0	12	5	0
2	B	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	4	0
4	B	7	0	0	1	0
All	All	7620	0	7629	520	1

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 34.

All (520) 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:400:THR:HG22	1:B:429:PHE:O	1.45	1.15
1:B:11:LYS:HA	1:B:14:ILE:HD12	1.22	1.13
1:A:44:ARG:HH11	1:A:44:ARG:HG3	0.93	1.08
1:A:54:ILE:H	1:A:54:ILE:HD12	0.95	1.08
1:B:135:LEU:CD1	1:B:140:LYS:HG3	1.85	1.06
1:B:119:MSE:HA	1:B:119:MSE:HE2	1.34	1.06
1:A:44:ARG:CG	1:A:44:ARG:HH11	1.69	1.04
1:A:305:HIS:HD2	1:A:311:PRO:HG3	1.19	1.03
1:A:54:ILE:H	1:A:54:ILE:CD1	1.68	1.03
1:A:112:ASN:HB2	1:A:200:ASN:HD21	1.25	1.01
1:B:106:PHE:HD2	1:B:195:VAL:HG11	1.26	1.00
1:A:305:HIS:CD2	1:A:311:PRO:HG3	1.99	0.98
1:A:44:ARG:HG3	1:A:44:ARG:NH1	1.72	0.98
1:B:119:MSE:CE	1:B:134:VAL:HG21	1.93	0.98
1:A:124:MSE:HE1	1:A:300:ALA:HB1	1.45	0.97
1:B:125:LEU:CD2	1:B:304:LEU:HD21	1.93	0.97
1:B:399:THR:HG21	1:B:431:ARG:HA	1.47	0.97
1:B:135:LEU:HD12	1:B:140:LYS:HG3	1.45	0.96
1:A:54:ILE:N	1:A:54:ILE:HD12	1.80	0.96
1:B:154:PRO:O	1:B:187:ARG:HD3	1.65	0.95
1:B:125:LEU:HD21	1:B:304:LEU:HD21	1.48	0.93
1:B:327:ARG:HH11	1:B:327:ARG:HG2	1.35	0.92
1:A:398:LEU:HD11	1:A:419:ILE:HD11	1.51	0.91
1:B:119:MSE:HE1	1:B:134:VAL:HG21	1.52	0.91
1:B:132:GLY:HA3	1:B:173:PHE:CE1	2.05	0.91
1:B:360:ARG:NH1	1:B:367:VAL:HG12	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:HD22	1:B:64:VAL:CG1	2.02	0.89
1:A:106:PHE:CD2	1:A:195:VAL:HG11	2.08	0.89
1:A:236:GLU:HA	1:A:250:THR:CG2	2.03	0.89
1:B:344:ASP:OD1	1:B:345:PHE:N	2.05	0.89
1:B:11:LYS:HA	1:B:14:ILE:CD1	2.03	0.89
1:B:334:ALA:HB2	1:B:479:ILE:HD13	1.53	0.87
1:B:114:LYS:HB3	1:B:177:GLU:HG3	1.54	0.87
1:B:204:ASP:HB3	1:B:206:LEU:H	1.38	0.87
1:B:409:GLU:O	1:B:413:GLU:OE1	1.94	0.86
1:A:68:VAL:HG11	1:A:72:ILE:HG12	1.56	0.85
1:B:399:THR:HG23	1:B:428:LEU:O	1.77	0.84
1:B:124:MSE:HE3	1:B:301:ILE:HD13	1.57	0.84
1:B:123:HIS:HE1	1:B:320:THR:HG23	1.40	0.84
1:B:7:VAL:O	1:B:11:LYS:HB3	1.78	0.84
1:B:124:MSE:CE	1:B:301:ILE:HD13	2.07	0.83
1:B:334:ALA:HB2	1:B:479:ILE:CD1	2.07	0.83
1:B:119:MSE:HA	1:B:119:MSE:CE	2.07	0.83
1:B:106:PHE:CD2	1:B:195:VAL:HG11	2.12	0.83
1:B:400:THR:CG2	1:B:429:PHE:O	2.28	0.82
1:B:329:GLU:OE2	1:B:472:ARG:HD2	1.80	0.82
1:B:110:GLY:O	1:B:114:LYS:HD2	1.80	0.81
1:B:106:PHE:HD2	1:B:195:VAL:CG1	1.94	0.80
1:B:462:ASP:HB3	1:B:465:LYS:HB2	1.63	0.80
1:A:235:ASN:HB3	1:A:238:LEU:HD12	1.65	0.79
1:B:201:ILE:HG21	1:B:238:LEU:HD21	1.64	0.79
1:A:453:ARG:NH2	1:A:469:PHE:O	2.16	0.79
1:B:384:MSE:O	1:B:388:VAL:HG23	1.83	0.79
1:B:360:ARG:NH1	1:B:367:VAL:CG1	2.45	0.78
1:B:119:MSE:HE3	1:B:134:VAL:HG21	1.65	0.78
1:B:125:LEU:HB3	1:B:130:GLU:HG2	1.65	0.78
1:A:416:ILE:HA	1:A:419:ILE:HD12	1.65	0.77
1:A:245:LYS:HG3	1:A:245:LYS:O	1.85	0.77
1:A:397:ILE:HD12	1:A:438:ALA:HB2	1.67	0.77
1:B:360:ARG:HH11	1:B:367:VAL:CG1	1.98	0.77
1:A:337:ILE:HG22	1:A:338:GLY:N	1.99	0.76
1:A:383:PRO:O	1:A:418:GLY:HA3	1.86	0.76
1:A:26:THR:HG22	1:A:38:GLY:C	2.05	0.76
1:A:143:LEU:HD11	1:A:169:GLY:HA3	1.68	0.75
1:A:289:ILE:HG21	1:A:362:ILE:HD12	1.68	0.75
1:A:337:ILE:HD12	1:A:479:ILE:HG12	1.69	0.75
1:A:112:ASN:HB2	1:A:200:ASN:ND2	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:VAL:HG13	1:B:148:TYR:HE1	1.52	0.74
1:A:185:GLN:O	1:A:186:GLN:HB2	1.85	0.74
1:B:38:GLY:HA2	1:B:64:VAL:HG23	1.68	0.74
1:B:11:LYS:CA	1:B:14:ILE:HD12	2.10	0.74
1:B:143:LEU:HG	1:B:144:GLY:H	1.51	0.74
1:A:123:HIS:O	1:A:127:SER:HB2	1.88	0.74
1:A:114:LYS:HE2	2:A:1486:ADP:O2B	1.87	0.74
1:B:292:PHE:HD1	1:B:293:ASN:N	1.85	0.73
1:A:140:LYS:HB2	1:A:151:ILE:HD13	1.69	0.73
1:B:110:GLY:O	1:B:114:LYS:CD	2.37	0.73
1:B:292:PHE:CD1	1:B:293:ASN:N	2.56	0.73
1:A:38:GLY:HA2	1:A:64:VAL:HG23	1.71	0.73
1:A:368:ILE:HG12	1:A:395:VAL:HB	1.71	0.72
1:B:148:TYR:O	1:B:149:ASP:HB2	1.89	0.72
1:A:106:PHE:HD2	1:A:195:VAL:HG11	1.54	0.71
1:A:146:SER:O	1:A:148:TYR:N	2.24	0.71
1:A:106:PHE:CD2	1:A:195:VAL:CG1	2.73	0.71
1:B:413:GLU:O	1:B:417:LYS:HG3	1.91	0.70
1:A:314:LEU:O	1:A:317:SER:HB2	1.92	0.70
1:B:472:ARG:O	1:B:476:GLU:HG2	1.92	0.70
1:B:267:SER:C	1:B:269:GLU:H	1.93	0.70
1:A:56:PRO:O	1:A:60:GLU:OE1	2.10	0.70
1:A:162:ALA:HA	1:A:165:GLU:OE1	1.91	0.69
1:A:130:GLU:HG3	1:A:131:ARG:H	1.56	0.69
1:A:301:ILE:O	1:A:305:HIS:HB3	1.92	0.69
1:B:157:ILE:O	1:B:161:SER:HB2	1.91	0.69
1:B:106:PHE:CD2	1:B:195:VAL:CG1	2.74	0.69
1:B:334:ALA:CB	1:B:479:ILE:HD13	2.22	0.69
1:B:111:THR:HG21	1:B:202:SER:HB3	1.74	0.69
1:B:193:PHE:O	1:B:226:LEU:HD12	1.93	0.68
1:B:121:ILE:HD11	1:B:197:ILE:HD11	1.76	0.68
1:B:427:VAL:O	1:B:427:VAL:HG22	1.93	0.68
1:B:139:VAL:HG13	1:B:148:TYR:CE1	2.27	0.68
1:B:317:SER:O	1:B:320:THR:HG22	1.94	0.68
1:B:125:LEU:HD23	1:B:304:LEU:HD21	1.75	0.68
1:B:17:VAL:HG22	1:B:17:VAL:O	1.95	0.67
1:B:265:GLU:OE1	1:B:272:GLN:HB3	1.94	0.67
1:B:303:ALA:O	1:B:307:LEU:HD13	1.95	0.67
1:A:94:LEU:O	1:A:97:GLU:N	2.27	0.67
1:B:111:THR:OG1	1:B:201:ILE:HA	1.94	0.67
1:A:124:MSE:HE3	1:A:304:LEU:CD2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ALA:O	1:B:243:ASN:N	2.29	0.66
1:A:6:ILE:HG22	1:A:7:VAL:N	2.09	0.66
1:B:96:PHE:O	1:B:97:GLU:HB2	1.96	0.66
1:B:277:THR:OG1	1:B:278:PRO:HD2	1.96	0.66
1:A:336:LYS:HB3	1:A:483:LEU:HD11	1.78	0.66
1:A:124:MSE:HE3	1:A:304:LEU:HD22	1.77	0.66
1:A:16:GLU:OE2	1:A:18:ARG:HD2	1.95	0.66
1:B:112:ASN:HD22	2:B:1486:ADP:H5'1	1.61	0.66
1:B:255:LYS:HA	1:B:260:ARG:HD2	1.77	0.65
1:A:59:MSE:HE2	1:A:76:PHE:CD1	2.31	0.65
1:A:130:GLU:HG3	1:A:131:ARG:N	2.10	0.65
1:A:16:GLU:OE2	1:A:18:ARG:NH1	2.18	0.65
1:A:20:PRO:C	1:A:22:ASP:H	2.00	0.65
1:B:327:ARG:NH1	1:B:327:ARG:HG2	2.06	0.64
1:A:17:VAL:HG13	1:A:79:ILE:HD13	1.80	0.64
1:B:142:ILE:HD12	1:B:147:TYR:HD2	1.61	0.64
1:B:15:LEU:HD22	1:B:80:GLN:HG2	1.79	0.64
1:B:86:TYR:CZ	1:B:90:LYS:HE3	2.33	0.64
1:B:51:SER:O	1:B:54:ILE:HG12	1.97	0.64
1:B:135:LEU:HD11	1:B:140:LYS:HG3	1.79	0.64
1:B:263:ASN:O	1:B:273:PHE:HA	1.98	0.63
1:A:236:GLU:HA	1:A:250:THR:HG21	1.79	0.63
1:B:142:ILE:HG22	1:B:143:LEU:H	1.63	0.63
1:B:38:GLY:HA2	1:B:64:VAL:CG2	2.28	0.63
1:A:140:LYS:CB	1:A:151:ILE:HD13	2.28	0.63
1:B:125:LEU:HD21	1:B:304:LEU:CD2	2.26	0.62
1:A:168:GLU:HG2	1:A:169:GLY:N	2.15	0.62
1:A:173:PHE:C	1:A:173:PHE:CD1	2.72	0.62
1:B:192:ARG:NH1	1:B:227:LYS:HA	2.14	0.62
1:B:140:LYS:HB2	1:B:151:ILE:HD13	1.82	0.62
1:B:103:VAL:HA	1:B:172:LYS:HG2	1.80	0.61
1:B:189:GLU:OE2	1:B:221:HIS:HE1	1.82	0.61
1:B:455:HIS:O	1:B:470:GLN:NE2	2.33	0.61
1:A:263:ASN:H	1:A:274:VAL:HG12	1.66	0.61
1:B:297:ALA:O	1:B:301:ILE:HG12	2.01	0.60
1:B:27:GLY:HA3	1:B:39:ASP:OD1	2.01	0.60
1:A:44:ARG:NH2	1:A:85:ARG:HG3	2.16	0.60
1:B:55:ILE:HB	1:B:56:PRO:HD3	1.83	0.60
1:A:463:GLU:CG	1:A:464:GLU:N	2.63	0.60
1:A:268:TRP:HA	1:A:362:ILE:HD11	1.83	0.60
1:B:333:GLY:O	1:B:336:LYS:HE3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ARG:HH12	1:B:478:ILE:HG12	1.67	0.60
1:A:367:VAL:O	1:A:367:VAL:HG23	2.02	0.60
1:A:44:ARG:CG	1:A:44:ARG:NH1	2.38	0.60
1:A:122:TYR:CD2	1:A:134:VAL:HB	2.36	0.60
1:B:110:GLY:HA2	1:B:198:PHE:HE1	1.67	0.60
1:B:142:ILE:CG2	1:B:143:LEU:N	2.64	0.59
1:A:305:HIS:HD2	1:A:311:PRO:CG	2.06	0.59
1:B:83:ASP:OD2	1:B:86:TYR:HB2	2.02	0.59
1:A:327:ARG:HD3	1:A:345:PHE:CE1	2.37	0.59
1:B:334:ALA:CB	1:B:479:ILE:CD1	2.78	0.59
1:A:361:LYS:N	4:A:2007:HOH:O	2.35	0.59
1:B:329:GLU:OE2	1:B:472:ARG:CD	2.50	0.59
1:B:403:PRO:O	1:B:461:ILE:O	2.21	0.59
1:A:271:THR:HB	1:A:286:THR:HG22	1.84	0.59
1:A:26:THR:CG2	1:A:38:GLY:HA3	2.33	0.59
1:A:387:GLU:O	1:A:391:LYS:HG2	2.02	0.58
1:B:453:ARG:NH2	1:B:469:PHE:O	2.36	0.58
1:A:17:VAL:HG13	1:A:79:ILE:CD1	2.34	0.58
1:A:339:LEU:HD21	1:A:442:ALA:HB3	1.86	0.58
1:B:399:THR:HG21	1:B:431:ARG:CA	2.28	0.58
1:B:140:LYS:HB3	1:B:147:TYR:O	2.03	0.57
1:A:480:ARG:HD3	1:B:172:LYS:HD2	1.86	0.57
1:B:426:LEU:HD21	1:B:428:LEU:HD11	1.85	0.57
1:B:130:GLU:O	1:B:131:ARG:HG3	2.04	0.57
1:A:22:ASP:O	1:A:24:GLU:N	2.37	0.57
1:B:142:ILE:HG22	1:B:143:LEU:N	2.19	0.57
1:B:134:VAL:HG22	1:B:135:LEU:N	2.19	0.57
1:B:198:PHE:CE2	1:B:238:LEU:HD13	2.39	0.57
1:A:336:LYS:HG2	1:B:308:GLY:O	2.04	0.57
1:A:339:LEU:HD23	1:A:448:VAL:HG23	1.87	0.57
1:A:463:GLU:CG	1:A:464:GLU:H	2.18	0.57
1:B:273:PHE:CE1	1:B:284:VAL:HB	2.40	0.57
1:B:136:THR:HG22	1:B:177:GLU:HB2	1.86	0.56
1:A:337:ILE:CD1	1:A:479:ILE:HG12	2.35	0.56
1:B:124:MSE:CE	1:B:314:LEU:HG	2.35	0.56
1:A:168:GLU:CG	1:A:169:GLY:N	2.69	0.56
1:B:131:ARG:HH21	1:B:143:LEU:HD13	1.71	0.56
1:B:249:ILE:HG13	1:B:306:GLN:NE2	2.21	0.56
1:B:9:ASN:CB	1:B:94:LEU:HD11	2.35	0.56
1:B:375:GLY:O	1:B:376:ASN:HB2	2.06	0.56
1:A:327:ARG:CD	1:A:345:PHE:CE1	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:GLU:HG2	1:A:464:GLU:H	1.71	0.56
1:B:338:GLY:HA2	1:B:444:ARG:HD2	1.87	0.56
1:B:432:ARG:HH12	1:B:478:ILE:CG1	2.17	0.56
1:B:123:HIS:CE1	1:B:320:THR:HG23	2.31	0.55
1:A:304:LEU:HB3	1:A:314:LEU:HD21	1.87	0.55
1:A:398:LEU:CD1	1:A:419:ILE:HD11	2.31	0.55
1:A:114:LYS:HB3	1:A:177:GLU:HG3	1.88	0.55
1:B:304:LEU:HB3	1:B:314:LEU:HD21	1.89	0.55
1:A:194:ASP:OD1	1:A:227:LYS:HD2	2.06	0.55
1:A:40:LEU:HD11	1:A:67:VAL:HG23	1.89	0.55
1:A:236:GLU:CA	1:A:250:THR:CG2	2.82	0.55
1:A:464:GLU:O	1:A:465:LYS:HB2	2.07	0.55
1:B:202:SER:OG	1:B:204:ASP:HB2	2.05	0.55
1:A:432:ARG:NH1	1:A:474:VAL:HG13	2.21	0.55
1:A:135:LEU:HD22	1:A:174:PHE:HZ	1.72	0.54
1:A:248:LYS:O	1:A:249:ILE:HD13	2.08	0.54
1:A:290:GLY:O	1:A:293:ASN:HB2	2.07	0.54
1:A:2:ASN:HB3	1:A:4:SER:H	1.72	0.54
1:B:125:LEU:CD2	1:B:304:LEU:CD2	2.78	0.54
1:A:35:VAL:HG21	1:A:61:LYS:HB2	1.90	0.54
1:B:462:ASP:O	1:B:463:GLU:C	2.45	0.54
1:A:267:SER:C	1:A:362:ILE:HD11	2.28	0.54
1:B:27:GLY:HA2	1:B:95:PHE:CZ	2.43	0.54
1:B:105:THR:HG22	1:B:193:PHE:CD1	2.43	0.54
1:A:23:LEU:O	1:A:24:GLU:C	2.45	0.54
1:A:68:VAL:HG11	1:A:72:ILE:CG1	2.32	0.54
1:A:74:LEU:O	1:A:76:PHE:N	2.41	0.54
1:A:97:GLU:HA	1:A:97:GLU:OE1	2.07	0.54
1:B:122:TYR:C	1:B:122:TYR:CD1	2.81	0.54
1:B:233:VAL:HG21	1:B:303:ALA:HB2	1.90	0.54
1:B:236:GLU:HA	1:B:250:THR:CG2	2.38	0.54
1:A:185:GLN:O	1:A:186:GLN:CB	2.55	0.54
1:B:140:LYS:HD2	1:B:151:ILE:HG21	1.89	0.53
1:A:114:LYS:CE	2:A:1486:ADP:O2B	2.56	0.53
1:B:55:ILE:HB	1:B:56:PRO:CD	2.38	0.53
1:B:125:LEU:O	1:B:128:LEU:N	2.40	0.53
1:B:23:LEU:HD22	1:B:64:VAL:HG13	1.84	0.53
1:B:159:ILE:O	1:B:163:MSE:HG3	2.08	0.53
1:A:245:LYS:CG	1:A:245:LYS:O	2.55	0.53
1:A:328:PHE:CE2	1:A:355:LEU:HD12	2.44	0.53
1:B:264:ILE:HG23	1:B:264:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:VAL:O	1:B:325:GLU:C	2.47	0.53
1:A:463:GLU:HG3	1:A:464:GLU:N	2.24	0.53
1:B:267:SER:C	1:B:269:GLU:N	2.62	0.53
1:B:267:SER:O	1:B:269:GLU:N	2.42	0.53
1:B:476:GLU:HA	1:B:479:ILE:HD12	1.90	0.52
1:A:57:GLU:O	1:A:61:LYS:HG3	2.09	0.52
1:B:305:HIS:C	1:B:307:LEU:H	2.13	0.52
1:B:285:PHE:CD2	1:B:319:GLU:HG3	2.45	0.52
1:A:462:ASP:HB2	1:A:465:LYS:HB3	1.91	0.52
1:A:129:GLY:O	1:A:130:GLU:HB2	2.10	0.52
1:A:470:GLN:HE21	1:A:472:ARG:HD3	1.74	0.52
1:B:23:LEU:HD22	1:B:64:VAL:HG11	1.88	0.52
1:A:141:ARG:HG2	1:A:146:SER:HB3	1.91	0.52
1:A:251:PHE:HA	1:A:259:TYR:O	2.09	0.52
1:A:306:GLN:O	1:A:307:LEU:HD23	2.10	0.52
1:A:26:THR:HG22	1:A:38:GLY:CA	2.40	0.52
1:B:3:ILE:CD1	1:B:23:LEU:HB2	2.39	0.52
1:B:334:ALA:HB2	1:B:479:ILE:HD11	1.89	0.52
1:B:3:ILE:O	1:B:7:VAL:HG23	2.10	0.52
1:B:84:SER:O	1:B:87:PHE:HB3	2.10	0.52
1:A:140:LYS:HB2	1:A:151:ILE:CD1	2.38	0.52
1:A:360:ARG:HG3	4:A:2007:HOH:O	2.10	0.52
1:A:203:ARG:HG2	1:A:212:PHE:CE1	2.45	0.52
1:A:272:GLN:HE22	1:A:283:LYS:HE3	1.73	0.52
1:A:354:LYS:HE3	2:A:1486:ADP:H1'	1.91	0.52
1:A:356:LEU:O	1:A:359:VAL:HG22	2.10	0.51
1:B:272:GLN:HG3	1:B:285:PHE:HB2	1.92	0.51
1:B:372:GLY:HA3	1:B:401:ASP:HB2	1.92	0.51
1:B:427:VAL:O	1:B:427:VAL:CG2	2.58	0.51
1:A:410:GLN:O	1:A:410:GLN:HG2	2.09	0.51
1:B:133:SER:HB2	1:B:142:ILE:O	2.11	0.51
1:B:221:HIS:HD2	1:B:224:ASP:HB2	1.76	0.51
1:B:409:GLU:C	1:B:413:GLU:OE1	2.47	0.51
1:B:467:VAL:HB	1:B:468:PRO:CD	2.41	0.51
1:A:153:THR:HG23	1:A:153:THR:O	2.10	0.51
1:B:124:MSE:HE3	1:B:314:LEU:HG	1.91	0.51
1:A:195:VAL:HG23	1:A:231:VAL:HG13	1.93	0.51
1:B:198:PHE:CD2	1:B:238:LEU:HD13	2.45	0.51
1:B:143:LEU:HG	1:B:144:GLY:N	2.23	0.51
1:A:263:ASN:ND2	1:A:274:VAL:HG11	2.26	0.51
1:B:124:MSE:HE1	1:B:301:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:NH1	1:B:327:ARG:CG	2.72	0.50
1:B:455:HIS:O	1:B:456:GLU:C	2.50	0.50
1:B:180:SER:CB	1:B:219:LYS:HZ2	2.25	0.50
1:A:26:THR:HG21	1:A:38:GLY:HA3	1.93	0.50
1:A:124:MSE:CE	1:A:300:ALA:HB1	2.30	0.50
1:A:205:HIS:HA	1:A:208:PHE:CD2	2.47	0.50
1:A:327:ARG:HD3	1:A:345:PHE:CD1	2.46	0.50
1:B:255:LYS:HA	1:B:260:ARG:CD	2.41	0.50
1:B:444:ARG:HG2	4:B:2007:HOH:O	2.12	0.50
1:B:140:LYS:HD2	1:B:151:ILE:CG2	2.41	0.50
1:B:388:VAL:CG1	1:B:392:LEU:HD12	2.42	0.50
1:A:109:THR:HG23	1:A:198:PHE:HD1	1.77	0.50
1:A:109:THR:HG22	1:A:222:LEU:HD22	1.94	0.50
1:A:74:LEU:HD23	1:A:76:PHE:CE2	2.47	0.50
1:B:108:VAL:HG22	1:B:197:ILE:HB	1.94	0.50
1:B:100:TRP:HB3	1:B:163:MSE:HE1	1.94	0.49
1:B:178:VAL:O	1:B:178:VAL:HG12	2.10	0.49
1:A:259:TYR:OH	1:A:305:HIS:ND1	2.43	0.49
1:B:205:HIS:HA	1:B:208:PHE:CD2	2.47	0.49
1:A:188:VAL:O	1:A:188:VAL:HG22	2.12	0.49
1:B:20:PRO:O	1:B:22:ASP:N	2.45	0.49
1:B:407:ASP:HB3	1:B:410:GLN:HG3	1.95	0.49
1:B:188:VAL:HG11	1:B:193:PHE:HZ	1.77	0.49
1:B:254:SER:O	1:B:260:ARG:HD2	2.12	0.49
1:B:362:ILE:HG12	1:B:362:ILE:O	2.11	0.49
1:A:268:TRP:N	1:A:362:ILE:HD11	2.28	0.49
1:A:70:ARG:CG	1:A:71:GLU:N	2.76	0.49
1:A:188:VAL:HG21	1:A:193:PHE:HZ	1.78	0.48
1:A:360:ARG:HB3	4:A:2007:HOH:O	2.12	0.48
1:A:26:THR:HG22	1:A:38:GLY:HA3	1.94	0.48
1:A:69:GLU:CD	1:A:84:SER:HB2	2.33	0.48
1:B:212:PHE:O	1:B:215:TYR:HB3	2.12	0.48
1:A:133:SER:HB2	1:A:166:ASN:OD1	2.13	0.48
1:A:480:ARG:HD3	1:B:172:LYS:CD	2.43	0.48
1:B:55:ILE:CD1	1:B:66:VAL:HG11	2.43	0.48
1:B:15:LEU:HD22	1:B:80:GLN:CG	2.43	0.48
1:A:1:MSE:CE	1:A:95:PHE:HA	2.43	0.48
1:A:379:ARG:HH22	1:A:410:GLN:HE21	1.61	0.48
1:A:69:GLU:HG3	1:A:84:SER:HB2	1.94	0.48
1:B:188:VAL:HG12	1:B:188:VAL:O	2.14	0.48
1:A:431:ARG:CZ	1:A:453:ARG:HD3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MSE:HE2	1:A:76:PHE:HD1	1.76	0.48
1:A:384:MSE:O	1:A:388:VAL:HG23	2.14	0.48
1:A:41:PHE:HD2	1:A:66:VAL:HG23	1.79	0.48
1:A:74:LEU:C	1:A:76:PHE:H	2.17	0.48
1:B:50:ASP:O	1:B:51:SER:C	2.52	0.48
1:A:134:VAL:HG22	1:A:135:LEU:N	2.28	0.48
1:A:400:THR:CG2	1:A:429:PHE:O	2.62	0.48
1:B:143:LEU:CG	1:B:144:GLY:N	2.77	0.48
1:A:13:LEU:HD12	1:A:13:LEU:N	2.28	0.48
1:A:55:ILE:N	1:A:56:PRO:HD2	2.28	0.48
1:A:69:GLU:CG	1:A:84:SER:HB2	2.44	0.48
1:B:208:PHE:CZ	1:B:212:PHE:HA	2.49	0.48
1:A:7:VAL:O	1:A:11:LYS:HB3	2.13	0.48
1:A:198:PHE:CD2	1:A:238:LEU:HD13	2.49	0.48
1:B:179:SER:HB2	1:B:182:ALA:H	1.79	0.48
1:A:267:SER:OG	1:A:269:GLU:HG2	2.14	0.47
1:B:329:GLU:CD	1:B:472:ARG:HD2	2.35	0.47
1:B:14:ILE:HG22	1:B:15:LEU:N	2.29	0.47
1:B:339:LEU:HG	1:B:339:LEU:H	1.50	0.47
1:A:86:TYR:OH	1:A:90:LYS:HE3	2.14	0.47
1:B:375:GLY:O	1:B:404:ARG:NH1	2.48	0.47
1:A:6:ILE:HG22	1:A:7:VAL:H	1.76	0.47
1:A:70:ARG:CG	1:A:71:GLU:H	2.28	0.47
1:B:112:ASN:HB2	1:B:200:ASN:HD21	1.78	0.47
1:A:342:VAL:HB	1:A:449:VAL:HG22	1.97	0.47
1:B:236:GLU:HA	1:B:250:THR:HG23	1.96	0.47
1:B:291:ASP:OD1	1:B:291:ASP:N	2.48	0.46
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.65	0.46
1:A:366:ARG:HG2	1:A:394:ASP:OD2	2.14	0.46
1:B:282:LEU:HD23	1:B:283:LYS:N	2.30	0.46
1:B:345:PHE:CG	1:B:346:ALA:N	2.84	0.46
1:B:110:GLY:HA2	1:B:198:PHE:CE1	2.50	0.46
1:B:259:TYR:CE2	1:B:302:ALA:HA	2.50	0.46
1:B:3:ILE:HG22	1:B:3:ILE:O	2.14	0.46
1:A:382:ARG:HB2	1:A:383:PRO:HD3	1.97	0.46
1:A:81:VAL:HG11	1:A:87:PHE:CG	2.50	0.46
1:A:68:VAL:HG21	1:A:72:ILE:HD11	1.98	0.46
1:B:198:PHE:HB3	1:B:234:LEU:CD2	2.45	0.46
1:B:208:PHE:HZ	1:B:212:PHE:HA	1.80	0.46
1:B:360:ARG:HH11	1:B:367:VAL:HG11	1.80	0.46
1:A:143:LEU:HB3	1:A:144:GLY:H	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG22	1:A:261:LEU:O	2.16	0.46
1:A:268:TRP:CA	1:A:362:ILE:HD11	2.44	0.46
1:A:462:ASP:O	1:A:463:GLU:C	2.54	0.46
1:B:285:PHE:CE2	1:B:319:GLU:HG3	2.51	0.46
1:B:100:TRP:HA	1:B:103:VAL:HG22	1.98	0.46
1:A:168:GLU:HG2	1:A:169:GLY:H	1.80	0.45
1:A:72:ILE:HA	1:A:72:ILE:HD13	1.88	0.45
1:B:152:THR:C	1:B:154:PRO:HD3	2.37	0.45
1:B:180:SER:HB3	1:B:219:LYS:NZ	2.30	0.45
1:B:399:THR:HG22	1:B:400:THR:N	2.31	0.45
1:B:404:ARG:CD	1:B:460:ILE:HD12	2.46	0.45
1:B:251:PHE:HA	1:B:259:TYR:O	2.16	0.45
1:A:153:THR:N	1:A:154:PRO:CD	2.79	0.45
1:A:307:LEU:O	1:A:309:TYR:N	2.49	0.45
1:B:305:HIS:C	1:B:307:LEU:N	2.70	0.45
1:B:384:MSE:HA	1:B:387:GLU:HB2	1.98	0.45
1:A:154:PRO:O	1:A:187:ARG:HD3	2.17	0.45
1:A:416:ILE:HA	1:A:419:ILE:CD1	2.40	0.45
1:B:301:ILE:HD11	1:B:318:LEU:CD1	2.46	0.45
1:B:74:LEU:O	1:B:76:PHE:N	2.49	0.45
1:B:287:ARG:HD3	1:B:332:ARG:NH2	2.31	0.45
1:B:339:LEU:HD22	1:B:442:ALA:HB1	1.99	0.45
1:B:45:ARG:HH12	1:B:186:GLN:HE22	1.63	0.45
1:A:192:ARG:HB3	1:A:227:LYS:HG2	1.98	0.45
1:A:305:HIS:C	1:A:305:HIS:ND1	2.69	0.45
1:B:383:PRO:O	1:B:418:GLY:HA3	2.17	0.45
1:B:115:THR:O	1:B:119:MSE:HG2	2.17	0.45
1:B:222:LEU:O	1:B:225:LEU:HB2	2.17	0.45
1:B:153:THR:N	1:B:154:PRO:HD3	2.32	0.45
1:A:398:LEU:HA	1:A:398:LEU:HD23	1.67	0.45
1:A:44:ARG:NH2	1:A:88:GLU:OE1	2.48	0.45
1:B:124:MSE:HE3	1:B:301:ILE:CD1	2.38	0.45
1:A:20:PRO:C	1:A:22:ASP:N	2.65	0.44
1:A:193:PHE:O	1:A:226:LEU:HD12	2.17	0.44
1:A:70:ARG:HG2	1:A:71:GLU:N	2.32	0.44
1:B:469:PHE:O	1:B:469:PHE:CD1	2.71	0.44
1:B:135:LEU:CD1	1:B:140:LYS:CG	2.77	0.44
1:B:336:LYS:HB3	1:B:483:LEU:HD11	1.99	0.44
1:A:104:LEU:O	1:A:173:PHE:HA	2.18	0.44
1:A:287:ARG:HD2	1:A:322:THR:HG22	2.00	0.44
1:A:360:ARG:HD3	1:A:360:ARG:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:TYR:CE1	1:B:189:GLU:HG2	2.52	0.44
1:A:122:TYR:O	1:A:126:THR:HG23	2.18	0.44
1:A:191:VAL:HG12	1:A:192:ARG:N	2.33	0.44
1:B:45:ARG:HG2	1:B:69:GLU:OE2	2.18	0.44
1:A:431:ARG:HD3	1:A:469:PHE:CE1	2.52	0.44
1:B:119:MSE:HE1	1:B:134:VAL:CG2	2.35	0.44
1:B:132:GLY:HA3	1:B:173:PHE:CD1	2.51	0.44
1:B:142:ILE:HD12	1:B:147:TYR:CD2	2.47	0.44
1:B:223:PHE:C	1:B:225:LEU:H	2.20	0.44
1:A:267:SER:HA	1:A:362:ILE:HG13	1.99	0.43
1:B:133:SER:CB	1:B:142:ILE:O	2.66	0.43
1:B:105:THR:HG22	1:B:193:PHE:HD1	1.83	0.43
1:B:180:SER:CB	1:B:219:LYS:NZ	2.80	0.43
1:B:59:MSE:HE2	1:B:76:PHE:HD2	1.83	0.43
1:B:104:LEU:HD11	1:B:307:LEU:HD23	1.98	0.43
1:B:3:ILE:HD11	1:B:23:LEU:HB2	2.00	0.43
1:B:323:GLY:C	1:B:324:VAL:CG2	2.86	0.43
1:B:268:TRP:CD1	1:B:362:ILE:HG12	2.53	0.43
1:A:26:THR:CG2	1:A:38:GLY:CA	2.96	0.43
1:A:73:ASP:O	1:A:74:LEU:HD12	2.18	0.43
1:B:20:PRO:C	1:B:22:ASP:H	2.20	0.43
1:B:353:GLU:OE2	1:B:357:LYS:HE2	2.19	0.43
1:B:480:ARG:O	1:B:482:LYS:N	2.51	0.43
1:B:119:MSE:CA	1:B:119:MSE:HE2	2.24	0.43
1:B:180:SER:HB3	1:B:219:LYS:HZ2	1.83	0.43
1:B:437:THR:O	1:B:441:ILE:HG23	2.18	0.43
1:A:120:MSE:O	1:A:124:MSE:HB2	2.19	0.43
1:A:26:THR:HG22	1:A:38:GLY:O	2.18	0.43
1:B:125:LEU:HD12	1:B:173:PHE:CE2	2.54	0.43
1:B:236:GLU:HG3	1:B:257:ALA:HB2	1.99	0.43
1:B:163:MSE:HE2	1:B:163:MSE:HB3	1.86	0.43
1:A:139:VAL:HG13	1:A:148:TYR:HE1	1.83	0.43
1:A:124:MSE:CE	1:A:304:LEU:HD22	2.48	0.43
1:B:421:LYS:H	1:B:421:LYS:HG2	1.67	0.43
1:B:42:ILE:HD13	1:B:88:GLU:HG3	2.00	0.43
1:A:189:GLU:OE2	1:A:221:HIS:NE2	2.45	0.43
1:B:263:ASN:O	1:B:273:PHE:CA	2.65	0.43
1:B:409:GLU:O	1:B:410:GLN:C	2.57	0.43
1:B:134:VAL:CG2	1:B:135:LEU:N	2.81	0.43
1:B:166:ASN:ND2	1:B:174:PHE:HB2	2.33	0.43
1:B:267:SER:O	1:B:289:ILE:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PHE:O	1:A:173:PHE:CD1	2.73	0.42
1:A:185:GLN:HB2	1:A:187:ARG:HG3	2.01	0.42
1:A:242:PHE:CD2	1:A:248:LYS:HD3	2.54	0.42
1:B:464:GLU:O	1:B:465:LYS:HG2	2.18	0.42
1:B:9:ASN:HB3	1:B:94:LEU:HD11	2.01	0.42
1:B:188:VAL:HG11	1:B:193:PHE:CZ	2.54	0.42
1:B:388:VAL:HG12	1:B:392:LEU:HD12	2.00	0.42
1:B:5:THR:O	1:B:9:ASN:HB2	2.19	0.42
1:A:305:HIS:ND1	1:A:305:HIS:O	2.53	0.42
1:A:356:LEU:HA	1:A:359:VAL:HG22	2.00	0.42
1:A:26:THR:CG2	1:A:38:GLY:C	2.82	0.42
1:A:369:VAL:CG1	1:A:396:VAL:HG22	2.49	0.42
1:B:426:LEU:CD2	1:B:428:LEU:HD11	2.47	0.42
1:B:38:GLY:CA	1:B:64:VAL:HG23	2.44	0.42
1:B:5:THR:HG22	1:B:9:ASN:ND2	2.33	0.42
1:A:112:ASN:HB3	2:A:1486:ADP:C4	2.54	0.42
1:A:431:ARG:NE	1:A:453:ARG:HD3	2.34	0.42
1:B:224:ASP:OD1	1:B:244:ARG:HG2	2.19	0.42
1:B:399:THR:HG22	1:B:400:THR:H	1.83	0.42
1:B:185:GLN:H	1:B:185:GLN:HG2	1.64	0.42
1:B:19:ALA:HA	1:B:20:PRO:HD2	1.88	0.42
1:A:256:ASN:OD1	1:A:256:ASN:N	2.53	0.42
1:B:91:VAL:HG12	1:B:92:ALA:N	2.35	0.42
1:A:305:HIS:CG	1:A:305:HIS:O	2.71	0.42
1:B:120:MSE:O	1:B:121:ILE:C	2.58	0.42
1:B:283:LYS:O	1:B:283:LYS:CG	2.67	0.42
1:B:15:LEU:HD22	1:B:80:GLN:CD	2.39	0.42
1:A:354:LYS:CE	2:A:1486:ADP:H1'	2.50	0.42
1:A:268:TRP:CE2	1:A:362:ILE:HG23	2.55	0.42
1:A:268:TRP:NE1	1:A:362:ILE:HG23	2.34	0.42
1:B:136:THR:O	1:B:151:ILE:HD12	2.20	0.42
1:B:399:THR:HA	1:B:428:LEU:O	2.20	0.42
1:A:121:ILE:HD11	1:A:197:ILE:CD1	2.49	0.42
1:A:201:ILE:HG23	1:A:201:ILE:O	2.20	0.42
1:A:67:VAL:HA	1:A:79:ILE:O	2.20	0.42
1:A:184:VAL:C	1:A:186:GLN:N	2.74	0.41
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.68	0.41
1:A:304:LEU:HA	1:A:304:LEU:HD12	1.47	0.41
1:B:124:MSE:HE1	1:B:301:ILE:HA	2.02	0.41
1:B:297:ALA:HB1	1:B:318:LEU:CD1	2.50	0.41
1:A:382:ARG:HB2	1:A:383:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ASP:O	1:A:404:ARG:N	2.53	0.41
1:A:124:MSE:HG2	1:A:317:SER:CB	2.50	0.41
1:A:25:ILE:HD12	1:A:40:LEU:HB2	2.02	0.41
1:B:287:ARG:HD2	1:B:322:THR:HG22	2.02	0.41
1:B:341:VAL:HG22	1:B:448:VAL:HB	2.03	0.41
1:A:366:ARG:HH21	1:A:368:ILE:HD11	1.85	0.41
1:B:234:LEU:N	1:B:249:ILE:O	2.52	0.41
1:B:14:ILE:HG22	1:B:15:LEU:H	1.85	0.41
1:B:282:LEU:HD23	1:B:283:LYS:H	1.84	0.41
1:B:360:ARG:HD2	1:B:360:ARG:HA	1.64	0.41
1:B:453:ARG:NH1	1:B:459:GLN:HA	2.36	0.41
1:A:305:HIS:C	1:A:307:LEU:H	2.22	0.41
1:B:234:LEU:HA	1:B:234:LEU:HD23	1.64	0.41
1:B:86:TYR:CE2	1:B:90:LYS:HE3	2.55	0.41
1:B:125:LEU:HD23	1:B:304:LEU:CD2	2.46	0.41
1:B:261:LEU:HA	1:B:274:VAL:O	2.20	0.41
1:B:35:VAL:HG22	1:B:35:VAL:O	2.21	0.41
1:B:383:PRO:O	1:B:387:GLU:HB2	2.20	0.41
1:A:101:LYS:HE2	1:A:101:LYS:HB2	1.77	0.41
1:A:249:ILE:HA	1:A:258:ASP:OD2	2.21	0.41
1:A:311:PRO:O	1:A:312:LYS:C	2.59	0.41
1:B:104:LEU:HA	1:B:194:ASP:OD2	2.21	0.41
1:A:125:LEU:HD13	1:A:173:PHE:CD2	2.55	0.41
1:A:238:LEU:O	1:A:239:ALA:C	2.57	0.41
1:A:91:VAL:O	1:A:92:ALA:C	2.58	0.41
1:B:289:ILE:HG21	1:B:362:ILE:HD12	2.03	0.41
1:A:366:ARG:NH2	1:A:368:ILE:HD11	2.36	0.41
1:B:248:LYS:HG3	1:B:248:LYS:O	2.21	0.41
1:B:297:ALA:HB1	1:B:318:LEU:HD13	2.03	0.41
1:A:90:LYS:HD3	1:A:90:LYS:HA	1.92	0.41
1:B:301:ILE:HD11	1:B:318:LEU:HD12	2.02	0.41
1:A:188:VAL:CG2	1:A:193:PHE:HZ	2.34	0.40
1:A:360:ARG:CB	4:A:2007:HOH:O	2.68	0.40
1:B:104:LEU:O	1:B:173:PHE:HA	2.21	0.40
1:B:317:SER:O	1:B:320:THR:CG2	2.66	0.40
1:B:462:ASP:CB	1:B:465:LYS:HB2	2.41	0.40
1:A:236:GLU:CA	1:A:250:THR:HG22	2.51	0.40
1:A:366:ARG:HB2	1:A:446:ASP:OD1	2.20	0.40
1:B:255:LYS:HE3	1:B:260:ARG:NH2	2.36	0.40
1:B:404:ARG:HG2	1:B:460:ILE:HD12	2.03	0.40
1:B:480:ARG:C	1:B:482:LYS:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLU:HA	1:A:250:THR:HG23	1.99	0.40
1:A:339:LEU:HD23	1:A:448:VAL:CG2	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLN:NE2	1:B:211:THR:OG1[5_664]	2.17	0.03

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	474/498 (95%)	395 (83%)	60 (13%)	19 (4%)	3	14
1	B	479/498 (96%)	377 (79%)	75 (16%)	27 (6%)	2	6
All	All	953/996 (96%)	772 (81%)	135 (14%)	46 (5%)	2	10

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	147	TYR
1	A	404	ARG
1	B	75	ASP
1	B	149	ASP
1	B	242	PHE
1	B	268	TRP
1	B	324	VAL
1	A	6	ILE
1	A	7	VAL
1	A	33	SER

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Mol	Chain	Res	Type
1	A	75	ASP
1	A	130	GLU
1	A	308	GLY
1	B	21	TYR
1	B	44	ARG
1	B	51	SER
1	B	61	LYS
1	B	97	GLU
1	B	129	GLY
1	B	306	GLN
1	B	325	GLU
1	B	471	ASP
1	B	481	ASP
1	A	143	LEU
1	A	281	LEU
1	A	346	ALA
1	A	465	LYS
1	B	34	LYS
1	B	224	ASP
1	B	262	GLY
1	B	456	GLU
1	B	480	ARG
1	B	484	LYS
1	A	129	GLY
1	A	204	ASP
1	A	242	PHE
1	A	338	GLY
1	B	20	PRO
1	B	376	ASN
1	B	463	GLU
1	A	91	VAL
1	B	121	ILE
1	B	222	LEU
1	B	337	ILE
1	A	121	ILE

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	407/416 (98%)	363 (89%)	44 (11%)	7	23
1	B	411/416 (99%)	359 (87%)	52 (13%)	5	15
All	All	818/832 (98%)	722 (88%)	96 (12%)	6	18

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	28	VAL
1	A	33	SER
1	A	44	ARG
1	A	54	ILE
1	A	74	LEU
1	A	84	SER
1	A	97	GLU
1	A	124	MSE
1	A	127	SER
1	A	131	ARG
1	A	142	ILE
1	A	143	LEU
1	A	145	ASN
1	A	152	THR
1	A	173	PHE
1	A	180	SER
1	A	183	LEU
1	A	195	VAL
1	A	202	SER
1	A	207	ASP
1	A	208	PHE
1	A	213	GLU
1	A	238	LEU
1	A	250	THR
1	A	254	SER
1	A	277	THR
1	A	287	ARG
1	A	289	ILE
1	A	304	LEU
1	A	305	HIS
1	A	314	LEU
1	A	328	PHE
1	A	362	ILE

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Mol	Chain	Res	Type
1	A	366	ARG
1	A	385	MSE
1	A	386	SER
1	A	413	GLU
1	A	421	LYS
1	A	426	LEU
1	A	427	VAL
1	A	447	SER
1	A	462	ASP
1	A	471	ASP
1	B	5	THR
1	B	8	SER
1	B	17	VAL
1	B	33	SER
1	B	36	LYS
1	B	51	SER
1	B	68	VAL
1	B	72	ILE
1	B	73	ASP
1	B	74	LEU
1	B	79	ILE
1	B	103	VAL
1	B	124	MSE
1	B	142	ILE
1	B	143	LEU
1	B	165	GLU
1	B	179	SER
1	B	180	SER
1	B	181	HIS
1	B	185	GLN
1	B	195	VAL
1	B	201	ILE
1	B	207	ASP
1	B	208	PHE
1	B	216	LEU
1	B	228	ASP
1	B	253	THR
1	B	261	LEU
1	B	265	GLU
1	B	273	PHE
1	B	275	LEU
1	B	277	THR

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Mol	Chain	Res	Type
1	B	282	LEU
1	B	324	VAL
1	B	327	ARG
1	B	328	PHE
1	B	332	ARG
1	B	339	LEU
1	B	342	VAL
1	B	347	HIS
1	B	348	SER
1	B	379	ARG
1	B	386	SER
1	B	391	LYS
1	B	399	THR
1	B	419	ILE
1	B	427	VAL
1	B	428	LEU
1	B	441	ILE
1	B	444	ARG
1	B	460	ILE
1	B	472	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	272	GLN
1	A	296	ASN
1	A	306	GLN
1	A	376	ASN
1	A	470	GLN
1	B	112	ASN
1	B	123	HIS
1	B	221	HIS
1	B	235	ASN
1	B	296	ASN
1	B	305	HIS
1	B	306	GLN
1	B	376	ASN

5.3.3 RNA [i](#)

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ADP	A	1486	3	25,29,29	1.02	2 (8%)	24,45,45	1.90	5 (20%)
2	ADP	B	1486	3	25,29,29	1.16	3 (12%)	24,45,45	1.87	5 (20%)

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	ADP	A	1486	3	-	0/12/32/32	0/3/3/3
2	ADP	B	1486	3	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1486	ADP	C2-N3	2.10	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1486	ADP	O4'-C1'	2.21	1.44	1.41
2	B	1486	ADP	O4'-C1'	2.59	1.44	1.41
2	A	1486	ADP	C5-C4	2.91	1.47	1.40
2	B	1486	ADP	C5-C4	3.53	1.48	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1486	ADP	N3-C2-N1	-6.27	123.40	128.86
2	B	1486	ADP	N3-C2-N1	-6.27	123.40	128.86
2	A	1486	ADP	C4-C5-N7	-3.43	106.09	109.41
2	B	1486	ADP	C4-C5-N7	-3.09	106.42	109.41
2	B	1486	ADP	C5'-C4'-C3'	-2.41	106.10	115.29
2	B	1486	ADP	O5'-C5'-C4'	-2.19	101.23	109.00
2	A	1486	ADP	O3B-PB-O2B	2.05	115.90	107.61
2	B	1486	ADP	O3B-PB-O2B	2.12	116.16	107.61
2	A	1486	ADP	C2'-C3'-C4'	2.35	107.19	102.62
2	A	1486	ADP	C4'-O4'-C1'	3.09	113.06	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1486	ADP	5	0
2	B	1486	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	469/498 (94%)	0.07	9 (1%) 67 64	67, 103, 151, 210	1 (0%)
1	B	474/498 (95%)	0.14	17 (3%) 43 37	72, 109, 151, 197	1 (0%)
All	All	943/996 (94%)	0.10	26 (2%) 53 48	67, 105, 151, 210	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	ILE	8.9
1	A	152	THR	8.7
1	B	207	ASP	6.5
1	A	207	ASP	5.3
1	A	153	THR	5.0
1	B	54	ILE	4.4
1	B	52	HIS	4.1
1	A	209	HIS	3.6
1	B	276	GLU	3.0
1	B	283	LYS	2.9
1	B	258	ASP	2.8
1	B	278	PRO	2.8
1	B	55	ILE	2.8
1	B	275	LEU	2.7
1	B	65	ALA	2.6
1	B	281	LEU	2.6
1	A	72	ILE	2.5
1	B	239	ALA	2.4
1	B	40	LEU	2.4
1	A	74	LEU	2.4
1	A	150	ASP	2.3
1	A	206	LEU	2.3
1	B	282	LEU	2.1
1	B	238	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	58	VAL	2.1
1	B	249	ILE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ADP	A	1486	27/27	0.96	0.25	1.85	92,116,141,168	0
2	ADP	B	1486	27/27	0.90	0.27	1.14	92,128,155,157	0
3	MG	B	1487	1/1	0.90	0.35	-	75,75,75,75	0
3	MG	A	1487	1/1	0.98	0.39	-	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.