



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:41 AM GMT

PDB ID : 3FMP  
Title : Crystal structure of the nucleoporin Nup214 in complex with the DEAD-box helicase Ddx19  
Authors : Napetschnig, J.; Debler, E.W.; Blobel, G.; Hoelz, A.  
Deposited on : 2008-12-22  
Resolution : 3.19 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

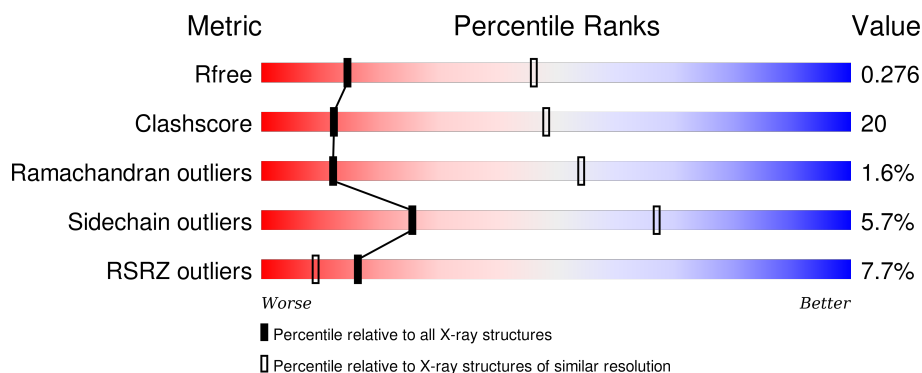
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	450	<div> <div>9%</div> <div>61%</div> <div>29%</div> <div>7%</div> </div>
1	C	450	<div> <div>8%</div> <div>60%</div> <div>31%</div> <div>7%</div> </div>
2	B	479	<div> <div>3%</div> <div>29%</div> <div>18%</div> <div>52%</div> </div>
2	D	479	<div> <div>2%</div> <div>28%</div> <div>19%</div> <div>52%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10216 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.

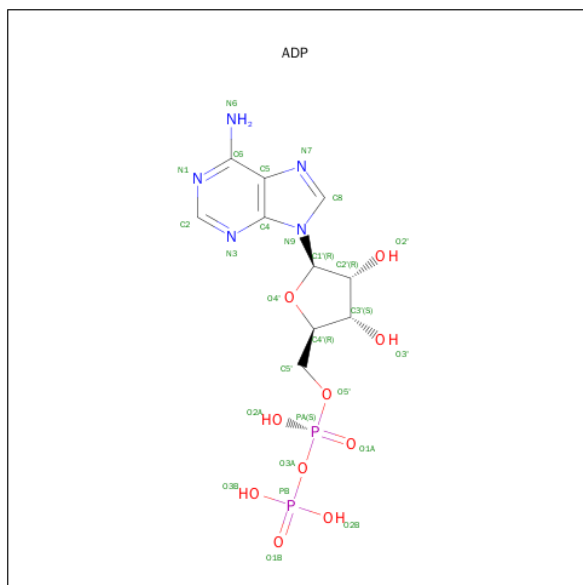
- Molecule 1 is a protein called Nuclear pore complex protein Nup214.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3274	2101	534	618	21			
1	C	420	Total	C	N	O	S	0	0	0
			3274	2101	534	618	21			

- Molecule 2 is a protein called ATP-dependent RNA helicase DDX19B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1807	1159	306	331	11			
2	D	229	Total	C	N	O	S	0	0	0
			1807	1159	306	331	11			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

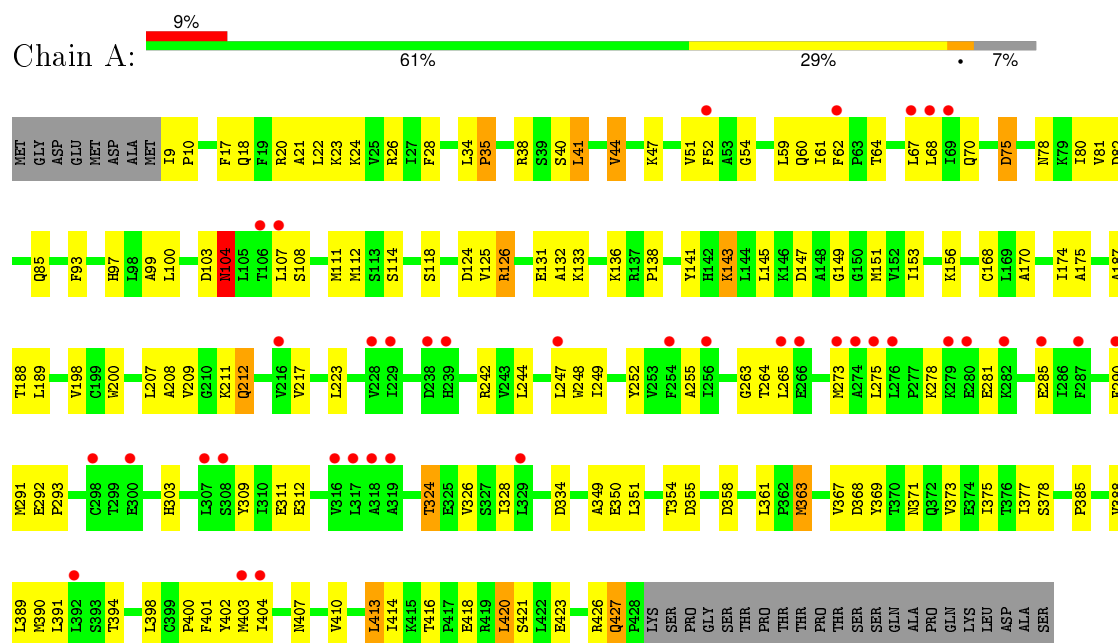


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

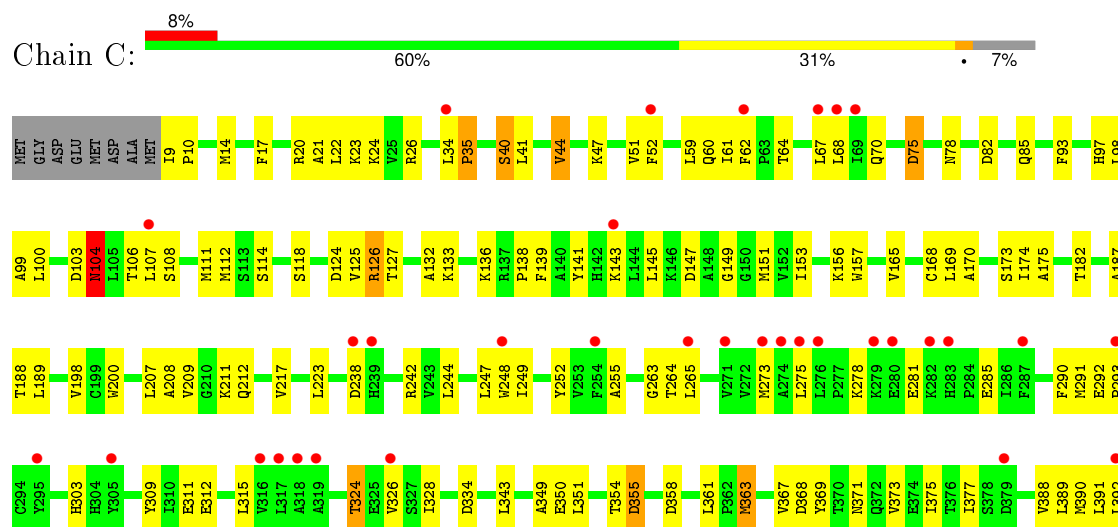
### 3 Residue-property plots

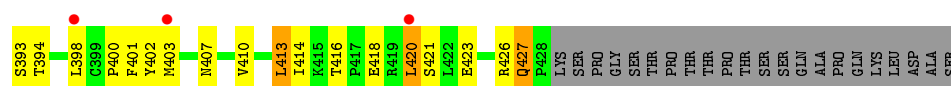
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Nuclear pore complex protein Nup214

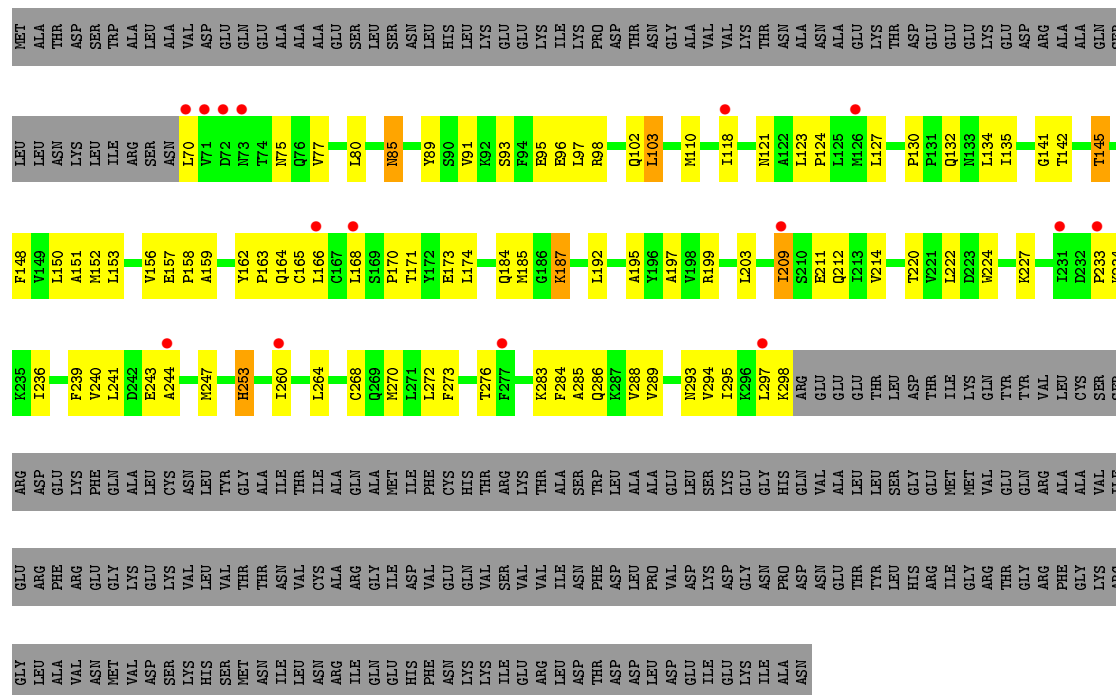
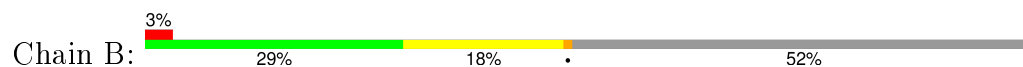


#### • Molecule 1: Nuclear pore complex protein Nup214

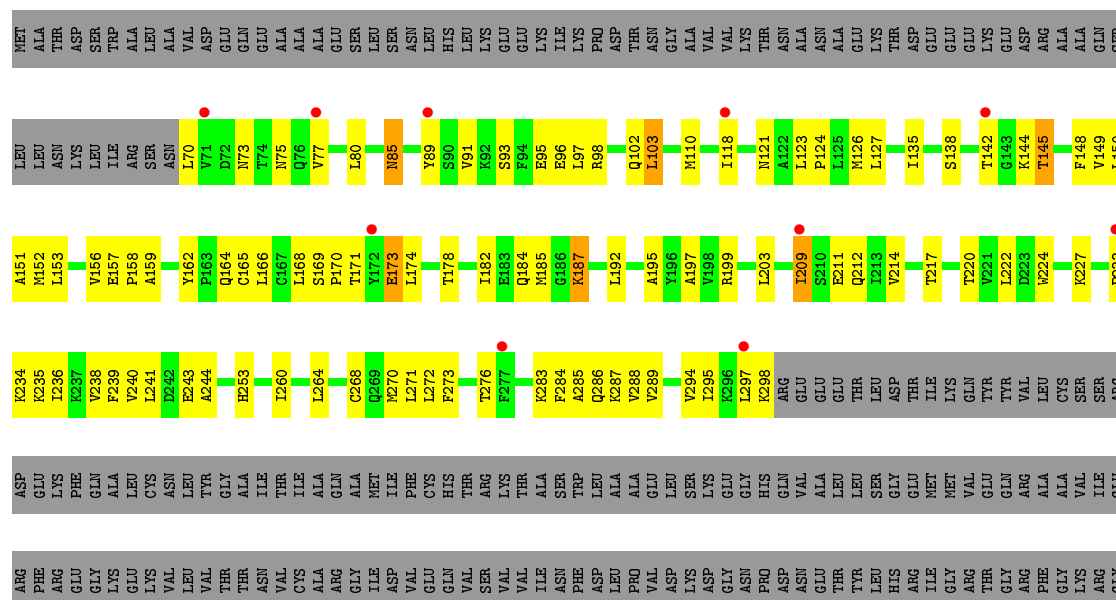
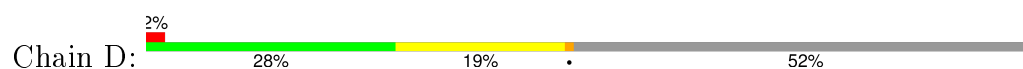




• Molecule 2: ATP-dependent RNA helicase DDX19B



• Molecule 2: ATP-dependent RNA helicase DDX19B



LEU	ALA	VAL	ASN	MET	VAL	ASP	SER	LYS	HIS	SER	MET	ASN	ILE	LEU	ASN	ARG	ILE	GLN	GLU	HIS	PHE	ASN	LYS	LYS	ILE	GLU	ARG	LEU	ASP	THR	ASP	ASP	LEU	ASP	GLU	ILE	GLU	LYS	ILE	ALA	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.37Å 112.92Å 142.57Å 90.00° 89.86° 90.00°	Depositor
Resolution (Å)	50.00 – 3.19 47.52 – 3.19	Depositor EDS
% Data completeness (in resolution range)	90.7 (50.00-3.19) 90.7 (47.52-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.249 , 0.283 0.250 , 0.276	Depositor DCC
$R_{free}$ test set	1504 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	92.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 84.2	EDS
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 29629 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.65	0/3351	0.74	0/4562
1	C	0.65	0/3351	0.75	0/4562
2	B	0.54	0/1842	0.68	0/2493
2	D	0.55	0/1842	0.69	0/2493
All	All	0.62	0/10386	0.72	0/14110

There are no bond length outliers.

There are no bond angle outliers.

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	3274	0	3301	120	0
1	C	3274	0	3301	122	0
2	B	1807	0	1868	81	0
2	D	1807	0	1868	86	0
3	B	27	0	12	4	0
3	D	27	0	12	3	0
All	All	10216	0	10362	405	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 20.

All (405) 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:369:TYR:CE1	1:A:413:LEU:HD22	1.99	0.98
1:C:369:TYR:CE1	1:C:413:LEU:HD22	2.04	0.92
2:B:239:PHE:CE2	2:B:241:LEU:HD11	2.07	0.90
1:A:52:PHE:CD1	1:A:107:LEU:HD13	2.07	0.89
1:A:44:VAL:HG23	1:A:51:VAL:HG22	1.56	0.87
2:D:239:PHE:CE2	2:D:241:LEU:HD11	2.09	0.87
2:B:98:ARG:HH22	1:C:145:LEU:HD13	1.42	0.84
1:C:52:PHE:CD1	1:C:107:LEU:HD13	2.11	0.84
1:C:44:VAL:HG23	1:C:51:VAL:HG22	1.58	0.83
1:C:112:MET:HE3	1:C:151:MET:HG2	1.60	0.83
1:C:99:ALA:HB3	1:C:108:SER:OG	1.79	0.82
1:C:407:ASN:O	1:C:410:VAL:HG22	1.83	0.79
1:A:407:ASN:O	1:A:410:VAL:HG22	1.82	0.79
1:C:390:MET:HE2	1:C:398:LEU:HD21	1.67	0.75
1:A:369:TYR:CD1	1:A:413:LEU:HD22	2.22	0.73
1:C:34:LEU:HD12	1:C:35:PRO:HD2	1.71	0.73
1:A:112:MET:HE3	1:A:151:MET:HG2	1.71	0.73
2:B:98:ARG:NH2	1:C:145:LEU:HD13	2.04	0.73
2:B:268:CYS:SG	2:B:270:MET:CE	2.77	0.73
1:A:34:LEU:HD12	1:A:35:PRO:HD2	1.71	0.72
1:A:255:ALA:HA	1:A:273:MET:HE2	1.69	0.72
1:C:255:ALA:HA	1:C:273:MET:HE2	1.72	0.71
1:A:390:MET:HE2	1:A:398:LEU:HD21	1.72	0.71
1:C:369:TYR:CD1	1:C:413:LEU:HD22	2.27	0.70
1:C:21:ALA:HB2	1:C:401:PHE:CD2	2.27	0.69
1:A:99:ALA:HB3	1:A:108:SER:OG	1.93	0.69
1:C:125:VAL:HG12	1:C:420:LEU:HD21	1.75	0.68
1:A:125:VAL:HG12	1:A:420:LEU:HD21	1.75	0.68
1:A:212:GLN:HE21	1:A:242:ARG:HD2	1.58	0.68
1:A:125:VAL:HG12	1:A:420:LEU:CD2	2.25	0.67
1:A:40:SER:O	1:A:41:LEU:HD23	1.94	0.67
1:C:153:ILE:HG21	1:C:170:ALA:HA	1.77	0.67
1:C:112:MET:CE	1:C:151:MET:HG2	2.25	0.66
2:D:268:CYS:SG	2:D:270:MET:CE	2.83	0.66
1:C:153:ILE:HG23	1:C:170:ALA:N	2.10	0.66
2:D:91:VAL:HG23	2:D:124:PRO:HG3	1.78	0.65
1:A:100:LEU:HD23	1:A:104:ASN:ND2	2.12	0.65
2:B:239:PHE:CZ	2:B:241:LEU:HD11	2.31	0.64
2:B:91:VAL:HG23	2:B:124:PRO:HG3	1.80	0.64
1:A:149:GLY:O	1:A:170:ALA:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:CE	1:A:151:MET:HG2	2.27	0.64
2:D:145:THR:HA	2:D:148:PHE:CE2	2.33	0.64
1:C:125:VAL:HG12	1:C:420:LEU:CD2	2.28	0.64
2:B:145:THR:HA	2:B:148:PHE:CE2	2.32	0.63
2:D:239:PHE:CZ	2:D:241:LEU:HD11	2.32	0.63
1:C:22:LEU:HD22	1:C:400:PRO:HB2	1.80	0.63
2:B:141:GLY:HA2	3:B:480:ADP:H5'1	1.80	0.63
2:B:168:LEU:HD11	2:B:260:ILE:HD12	1.80	0.63
1:A:20:ARG:NH1	1:A:377:ILE:HD12	2.14	0.63
1:A:153:ILE:HG21	1:A:170:ALA:HA	1.80	0.62
1:A:60:GLN:C	1:A:61:ILE:HD12	2.19	0.62
1:A:93:PHE:O	1:A:111:MET:HE3	1.99	0.62
1:C:211:LYS:NZ	1:C:217:VAL:HG21	2.15	0.62
2:D:233:PRO:HA	2:D:236:ILE:HD13	1.81	0.62
2:B:233:PRO:HA	2:B:236:ILE:HD13	1.82	0.61
2:B:91:VAL:HG13	2:B:96:GLU:OE1	2.00	0.61
2:B:135:ILE:HD13	2:B:285:ALA:HB1	1.83	0.61
2:B:103:LEU:HD21	2:B:150:LEU:HD23	1.83	0.61
1:C:93:PHE:O	1:C:111:MET:HE3	2.01	0.61
1:C:60:GLN:C	1:C:61:ILE:HD12	2.21	0.60
2:B:244:ALA:CB	2:B:272:LEU:HD21	2.31	0.60
2:D:135:ILE:HD13	2:D:285:ALA:HB1	1.82	0.60
2:D:91:VAL:HG13	2:D:96:GLU:OE1	2.02	0.60
2:B:158:PRO:HA	2:B:212:GLN:HE21	1.67	0.60
2:B:103:LEU:O	2:B:103:LEU:HD12	2.01	0.59
2:D:171:THR:OG1	2:D:174:LEU:HD13	2.02	0.59
1:A:21:ALA:HB2	1:A:401:PHE:CD2	2.38	0.59
2:B:195:ALA:HB3	2:B:214:VAL:HG22	1.84	0.59
1:A:20:ARG:NH1	1:A:377:ILE:CD1	2.66	0.59
2:D:158:PRO:HA	2:D:212:GLN:HE21	1.68	0.59
2:D:184:GLN:O	2:D:187:LYS:HB2	2.03	0.58
1:A:22:LEU:N	1:A:22:LEU:HD12	2.18	0.58
1:C:156:LYS:HD2	1:C:198:VAL:HG12	1.85	0.58
1:A:24:LYS:HZ1	1:A:78:ASN:HA	1.68	0.58
1:C:9:ILE:N	1:C:10:PRO:CD	2.67	0.58
1:C:68:LEU:HD21	1:C:388:VAL:HG11	1.85	0.58
1:A:391:LEU:O	1:A:398:LEU:HA	2.04	0.58
2:D:168:LEU:HD11	2:D:260:ILE:HD12	1.86	0.58
1:A:23:LYS:HZ1	1:A:75:ASP:HB3	1.69	0.58
2:D:103:LEU:O	2:D:103:LEU:HD12	2.04	0.57
2:D:209:ILE:HG23	2:D:211:GLU:OE1	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:PHE:CE2	2:B:241:LEU:CD1	2.85	0.57
2:D:103:LEU:HD21	2:D:150:LEU:HD23	1.84	0.57
1:C:21:ALA:HB2	1:C:401:PHE:CE2	2.39	0.57
1:A:153:ILE:HG23	1:A:170:ALA:N	2.19	0.57
2:B:171:THR:OG1	2:B:174:LEU:HD13	2.04	0.57
2:D:192:LEU:HA	2:D:212:GLN:HE22	1.68	0.57
2:B:152:MET:O	2:B:156:VAL:HG23	2.05	0.57
1:A:112:MET:HE2	1:A:118:SER:HB3	1.87	0.57
2:B:97:LEU:C	2:B:98:ARG:HG3	2.26	0.56
1:C:64:THR:HG21	1:C:368:ASP:OD1	2.05	0.56
2:D:244:ALA:CB	2:D:272:LEU:HD21	2.35	0.56
2:D:272:LEU:HD23	2:D:273:PHE:N	2.21	0.56
1:C:61:ILE:HD12	1:C:61:ILE:N	2.20	0.56
2:D:152:MET:HE2	2:D:165:CYS:HB3	1.86	0.56
2:D:244:ALA:HB2	2:D:272:LEU:HD21	1.88	0.56
1:A:9:ILE:N	1:A:10:PRO:CD	2.69	0.56
2:B:244:ALA:HB2	2:B:272:LEU:HD21	1.88	0.55
2:D:95:GLU:N	2:D:95:GLU:OE1	2.32	0.55
2:D:152:MET:O	2:D:156:VAL:HG23	2.05	0.55
2:B:268:CYS:SG	2:B:270:MET:HE1	2.46	0.55
1:A:427:GLN:N	1:A:427:GLN:HE21	2.04	0.55
1:A:64:THR:HG21	1:A:368:ASP:OD1	2.05	0.55
1:C:138:PRO:HG2	1:C:141:TYR:CZ	2.42	0.55
1:A:61:ILE:N	1:A:61:ILE:HD12	2.20	0.55
2:B:184:GLN:O	2:B:187:LYS:HB2	2.06	0.55
2:B:118:ILE:HB	2:B:142:THR:HG22	1.89	0.55
2:D:152:MET:CE	2:D:165:CYS:HB3	2.37	0.55
1:A:390:MET:CE	1:A:398:LEU:HD21	2.38	0.54
1:C:103:ASP:OD1	1:C:104:ASN:N	2.40	0.54
1:A:112:MET:CE	1:A:118:SER:HB3	2.37	0.54
1:C:208:ALA:HB2	1:C:248:TRP:CE3	2.43	0.54
1:A:212:GLN:NE2	1:A:242:ARG:HD2	2.22	0.54
1:A:249:ILE:HG23	1:A:309:TYR:CD2	2.43	0.54
2:B:95:GLU:OE1	2:B:95:GLU:N	2.37	0.54
2:D:70:LEU:HD11	3:D:480:ADP:C5	2.42	0.54
1:A:10:PRO:HD2	1:A:290:PHE:CE2	2.43	0.54
2:B:91:VAL:HG21	2:B:97:LEU:HD21	1.90	0.54
2:D:97:LEU:C	2:D:98:ARG:HG3	2.28	0.54
1:A:200:TRP:CD2	1:A:207:LEU:HD13	2.43	0.53
1:C:200:TRP:CD2	1:C:207:LEU:HD13	2.43	0.53
1:A:131:GLU:O	1:A:133:LYS:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ILE:HG23	1:C:309:TYR:CD2	2.43	0.53
1:C:174:ILE:CG2	1:C:189:LEU:HB2	2.39	0.53
1:A:208:ALA:HB2	1:A:248:TRP:CE3	2.44	0.53
2:D:270:MET:HB2	2:D:289:VAL:HG13	1.91	0.52
1:A:103:ASP:OD1	1:A:104:ASN:N	2.42	0.52
1:C:391:LEU:O	1:C:398:LEU:HA	2.10	0.52
2:D:239:PHE:CE2	2:D:241:LEU:CD1	2.90	0.52
2:D:118:ILE:HB	2:D:142:THR:HG22	1.91	0.52
2:D:195:ALA:HB3	2:D:214:VAL:HG22	1.91	0.52
1:C:153:ILE:CG2	1:C:170:ALA:HA	2.40	0.52
2:B:130:PRO:HD3	1:C:187:ALA:HB2	1.92	0.52
2:B:192:LEU:HA	2:B:212:GLN:HE22	1.73	0.52
1:A:52:PHE:CG	1:A:107:LEU:HD13	2.45	0.51
1:A:133:LYS:O	1:A:136:LYS:HD3	2.09	0.51
1:C:212:GLN:HE21	1:C:242:ARG:HD2	1.76	0.51
2:B:239:PHE:HB3	2:B:270:MET:HE2	1.91	0.51
1:C:22:LEU:HD12	1:C:22:LEU:N	2.25	0.51
2:D:197:ALA:HA	2:D:224:TRP:CZ2	2.45	0.51
2:D:240:VAL:O	2:D:241:LEU:HD12	2.10	0.51
1:C:208:ALA:HB2	1:C:248:TRP:CZ3	2.46	0.51
1:C:187:ALA:HB1	1:C:223:LEU:HD12	1.93	0.51
2:B:80:LEU:HB2	2:B:294:VAL:HB	1.93	0.51
1:C:124:ASP:OD2	1:C:126:ARG:NH1	2.43	0.51
1:C:9:ILE:N	1:C:10:PRO:HD2	2.25	0.51
1:C:124:ASP:OD1	1:C:126:ARG:N	2.44	0.51
1:C:10:PRO:HD2	1:C:290:PHE:CE2	2.46	0.51
1:A:138:PRO:HG2	1:A:141:TYR:CZ	2.46	0.51
2:B:156:VAL:HG22	2:B:165:CYS:SG	2.51	0.50
1:A:187:ALA:HB1	1:A:223:LEU:HD12	1.92	0.50
2:D:268:CYS:SG	2:D:270:MET:HE1	2.51	0.50
1:C:363:MET:HA	1:C:363:MET:HE3	1.93	0.50
1:A:108:SER:O	1:A:108:SER:OG	2.12	0.50
2:D:91:VAL:HG21	2:D:97:LEU:HD21	1.92	0.50
1:A:208:ALA:HB2	1:A:248:TRP:CZ3	2.46	0.50
2:B:75:ASN:HB2	2:B:298:LYS:O	2.11	0.50
2:B:197:ALA:HA	2:B:224:TRP:CZ2	2.47	0.50
1:C:291:MET:O	1:C:292:GLU:C	2.49	0.50
1:A:40:SER:O	1:A:97:HIS:HA	2.11	0.50
2:D:80:LEU:HB2	2:D:294:VAL:HB	1.93	0.50
1:C:326:VAL:HB	1:C:349:ALA:HB3	1.92	0.50
2:D:91:VAL:CG1	2:D:96:GLU:OE1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:CD2	1:A:104:ASN:ND2	2.74	0.50
1:C:363:MET:SD	1:C:394:THR:HG22	2.52	0.50
1:C:263:GLY:O	1:C:265:LEU:N	2.44	0.50
2:B:123:LEU:HB3	2:B:127:LEU:HD12	1.93	0.50
1:A:124:ASP:OD1	1:A:126:ARG:N	2.42	0.49
1:A:47:LYS:HG3	1:A:418:GLU:OE2	2.12	0.49
1:C:98:LEU:HD22	1:C:107:LEU:HD11	1.94	0.49
1:C:100:LEU:HD23	1:C:104:ASN:ND2	2.27	0.49
2:B:134:LEU:HD12	2:B:293:ASN:O	2.12	0.49
2:D:284:PHE:CE1	2:D:288:VAL:HG21	2.48	0.49
1:C:61:ILE:N	1:C:61:ILE:CD1	2.76	0.49
1:A:211:LYS:NZ	1:A:217:VAL:HG21	2.27	0.49
1:C:351:LEU:HD13	1:C:361:LEU:HA	1.93	0.49
1:C:23:LYS:HZ1	1:C:75:ASP:HB3	1.77	0.49
2:D:156:VAL:HG22	2:D:165:CYS:SG	2.52	0.49
2:B:91:VAL:CG1	2:B:96:GLU:OE1	2.61	0.49
1:A:59:LEU:HD12	1:A:60:GLN:H	1.77	0.49
2:D:173:GLU:O	2:D:174:LEU:HD12	2.13	0.49
2:B:152:MET:CE	2:B:165:CYS:HB3	2.42	0.49
2:B:70:LEU:HD11	3:B:480:ADP:C5	2.48	0.48
1:A:9:ILE:N	1:A:10:PRO:HD2	2.27	0.48
2:B:297:LEU:HD12	2:B:298:LYS:N	2.29	0.48
2:B:241:LEU:HD21	2:B:288:VAL:HG11	1.95	0.48
1:C:17:PHE:CE1	1:C:328:ILE:HD11	2.49	0.48
2:B:209:ILE:HG23	2:B:211:GLU:OE1	2.13	0.48
1:A:59:LEU:HD21	1:A:107:LEU:CD2	2.43	0.48
2:D:268:CYS:O	2:D:270:MET:HE3	2.13	0.48
1:A:174:ILE:CG2	1:A:189:LEU:HB2	2.43	0.48
1:A:61:ILE:N	1:A:61:ILE:CD1	2.76	0.48
2:B:152:MET:HE2	2:B:165:CYS:HB3	1.95	0.48
1:A:326:VAL:HB	1:A:349:ALA:HB3	1.95	0.48
1:C:133:LYS:O	1:C:136:LYS:HD3	2.13	0.48
2:B:272:LEU:HD23	2:B:273:PHE:N	2.28	0.48
1:C:309:TYR:CE2	1:C:311:GLU:HA	2.49	0.48
1:C:20:ARG:NH1	1:C:377:ILE:HD12	2.28	0.48
1:A:363:MET:HA	1:A:363:MET:HE3	1.95	0.48
1:C:21:ALA:HA	1:C:401:PHE:HA	1.95	0.48
2:D:75:ASN:HB2	2:D:298:LYS:O	2.14	0.48
1:A:263:GLY:O	1:A:265:LEU:N	2.47	0.48
2:D:239:PHE:HB3	2:D:270:MET:HE2	1.95	0.47
1:C:209:VAL:O	1:C:209:VAL:CG2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LYS:HZ1	1:C:78:ASN:HA	1.79	0.47
2:B:272:LEU:HB2	2:B:289:VAL:HG21	1.97	0.47
2:D:241:LEU:HD21	2:D:288:VAL:HG11	1.96	0.47
2:D:123:LEU:HB3	2:D:127:LEU:HD12	1.94	0.47
2:B:283:LYS:HA	2:B:286:GLN:HE21	1.79	0.47
1:C:24:LYS:NZ	1:C:78:ASN:HD22	2.12	0.47
1:A:52:PHE:CD1	1:A:107:LEU:CD1	2.91	0.47
1:A:351:LEU:HD13	1:A:361:LEU:HA	1.95	0.47
1:C:52:PHE:O	1:C:98:LEU:HD13	2.14	0.47
1:C:174:ILE:HG23	1:C:189:LEU:HB2	1.97	0.47
1:C:209:VAL:O	1:C:209:VAL:HG23	2.14	0.47
2:B:239:PHE:CG	2:B:264:LEU:HD11	2.49	0.47
1:C:108:SER:OG	1:C:108:SER:O	2.25	0.47
2:D:241:LEU:CD2	2:D:288:VAL:HG11	2.45	0.47
1:A:363:MET:SD	1:A:394:THR:HG22	2.54	0.47
2:D:283:LYS:HA	2:D:286:GLN:HE21	1.80	0.47
1:C:52:PHE:CG	1:C:107:LEU:HD13	2.47	0.47
2:D:192:LEU:HA	2:D:212:GLN:NE2	2.29	0.47
1:A:354:THR:N	1:A:358:ASP:O	2.39	0.47
1:C:59:LEU:HD12	1:C:60:GLN:H	1.79	0.47
2:B:70:LEU:HD21	3:B:480:ADP:C8	2.50	0.47
2:B:284:PHE:CE1	2:B:288:VAL:HG21	2.50	0.47
1:C:211:LYS:HZ1	1:C:217:VAL:HG21	1.78	0.47
2:D:138:SER:OG	2:D:144:LYS:HD2	2.14	0.47
1:A:375:ILE:HG12	1:A:402:TYR:CD2	2.50	0.47
2:B:157:GLU:OE2	2:B:159:ALA:HB3	2.15	0.47
1:C:59:LEU:HD21	1:C:107:LEU:CD2	2.45	0.46
2:B:135:ILE:CD1	2:B:285:ALA:HB1	2.45	0.46
2:D:297:LEU:HD12	2:D:298:LYS:N	2.30	0.46
1:A:17:PHE:CE1	1:A:328:ILE:HD11	2.50	0.46
1:C:175:ALA:CB	1:C:188:THR:HG22	2.46	0.46
2:D:85:ASN:ND2	2:D:85:ASN:N	2.63	0.46
2:D:148:PHE:O	2:D:151:ALA:HB3	2.16	0.46
1:A:200:TRP:CH2	1:A:207:LEU:HD22	2.50	0.46
1:A:124:ASP:OD2	1:A:126:ARG:NH1	2.48	0.46
1:C:24:LYS:CE	1:C:78:ASN:HA	2.46	0.46
2:D:222:LEU:HD12	2:D:222:LEU:O	2.16	0.46
1:A:209:VAL:HG23	1:A:209:VAL:O	2.14	0.46
1:C:200:TRP:CH2	1:C:207:LEU:HD22	2.50	0.46
1:A:156:LYS:HD2	1:A:198:VAL:HG12	1.98	0.46
1:C:367:VAL:HG22	1:C:403:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:LEU:HD21	1:C:303:HIS:HB2	1.98	0.46
2:B:91:VAL:HG12	2:B:93:SER:O	2.16	0.46
1:C:51:VAL:HG23	1:C:64:THR:OG1	2.16	0.46
1:A:24:LYS:CE	1:A:78:ASN:HA	2.46	0.46
1:A:24:LYS:NZ	1:A:78:ASN:HD22	2.14	0.46
1:A:67:LEU:C	1:A:68:LEU:HD12	2.36	0.46
1:C:62:PHE:HB2	1:C:67:LEU:HD11	1.97	0.46
2:B:239:PHE:CD1	2:B:264:LEU:HD11	2.51	0.46
1:C:20:ARG:NH1	1:C:377:ILE:CD1	2.79	0.46
2:B:268:CYS:SG	2:B:270:MET:HE2	2.55	0.46
2:B:123:LEU:N	2:B:124:PRO:CD	2.79	0.46
1:A:22:LEU:HD22	1:A:400:PRO:HB2	1.97	0.46
1:A:70:GLN:CG	1:A:402:TYR:OH	2.64	0.46
1:A:209:VAL:O	1:A:209:VAL:CG2	2.64	0.46
1:C:138:PRO:HG2	1:C:141:TYR:CE2	2.51	0.45
2:B:75:ASN:HB3	2:B:298:LYS:HB2	1.98	0.45
1:A:291:MET:O	1:A:292:GLU:C	2.54	0.45
1:C:375:ILE:HG12	1:C:402:TYR:CD2	2.50	0.45
1:C:40:SER:O	1:C:41:LEU:HD23	2.16	0.45
1:C:112:MET:CE	1:C:118:SER:HB3	2.45	0.45
1:A:104:ASN:HD22	1:A:104:ASN:HA	1.53	0.45
2:B:192:LEU:HA	2:B:212:GLN:NE2	2.32	0.45
1:C:23:LYS:HG2	1:C:23:LYS:HZ2	1.70	0.45
1:C:75:ASP:N	1:C:75:ASP:OD1	2.48	0.45
1:A:62:PHE:HB2	1:A:67:LEU:HD11	1.97	0.45
2:B:85:ASN:N	2:B:85:ASN:ND2	2.64	0.45
2:D:121:ASN:O	2:D:124:PRO:HD2	2.17	0.45
2:D:85:ASN:HD22	2:D:85:ASN:H	1.65	0.45
1:A:75:ASP:OD1	1:A:75:ASP:N	2.49	0.45
2:B:110:MET:SD	2:B:185:MET:HE3	2.57	0.45
1:C:324:THR:O	1:C:350:GLU:HA	2.16	0.45
1:A:64:THR:HG21	1:A:368:ASP:CG	2.37	0.45
1:A:68:LEU:HD21	1:A:388:VAL:HG11	1.98	0.45
1:C:361:LEU:O	1:C:393:SER:HA	2.17	0.45
1:A:28:PHE:CZ	1:A:54:GLY:O	2.70	0.45
1:C:312:GLU:CD	1:C:312:GLU:H	2.20	0.45
2:D:77:VAL:CG1	2:D:295:ILE:HG23	2.47	0.45
1:A:100:LEU:HD23	1:A:104:ASN:HD21	1.81	0.44
1:A:371:ASN:O	1:A:414:ILE:HD12	2.16	0.44
2:B:270:MET:HB2	2:B:289:VAL:HG13	1.98	0.44
2:D:240:VAL:C	2:D:241:LEU:HD12	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:CG2	1:A:170:ALA:HA	2.44	0.44
2:B:148:PHE:O	2:B:151:ALA:HB3	2.17	0.44
2:D:148:PHE:O	2:D:149:VAL:C	2.56	0.44
1:A:367:VAL:HG22	1:A:403:MET:HE2	2.00	0.44
1:A:21:ALA:HB2	1:A:401:PHE:CE2	2.52	0.44
1:C:212:GLN:NE2	1:C:242:ARG:HD2	2.31	0.44
1:C:106:THR:O	1:C:106:THR:HG22	2.18	0.44
2:B:240:VAL:O	2:B:241:LEU:HD12	2.17	0.44
2:B:268:CYS:O	2:B:270:MET:HE3	2.18	0.44
2:D:123:LEU:N	2:D:124:PRO:CD	2.80	0.44
2:D:70:LEU:HD11	3:D:480:ADP:C6	2.53	0.44
1:C:157:TRP:HA	1:C:165:VAL:HG23	2.00	0.44
1:C:427:GLN:N	1:C:427:GLN:HE21	2.15	0.44
1:A:426:ARG:C	1:A:427:GLN:HE21	2.21	0.44
1:C:40:SER:O	1:C:97:HIS:HA	2.17	0.44
2:D:150:LEU:O	2:D:151:ALA:C	2.56	0.43
1:A:10:PRO:HD2	1:A:290:PHE:CZ	2.53	0.43
2:D:75:ASN:HB3	2:D:298:LYS:HB2	1.98	0.43
1:C:26:ARG:HB3	1:C:82:ASP:O	2.18	0.43
1:C:24:LYS:HZ3	1:C:78:ASN:HD22	1.65	0.43
2:B:153:LEU:HD11	2:B:185:MET:HB3	2.00	0.43
1:A:175:ALA:HB1	1:A:188:THR:HG22	2.00	0.43
2:B:222:LEU:HD12	2:B:222:LEU:O	2.17	0.43
1:C:326:VAL:HG21	1:C:389:LEU:HD21	2.00	0.43
2:B:203:LEU:CD1	2:B:209:ILE:HD11	2.48	0.43
1:A:312:GLU:CD	1:A:312:GLU:H	2.21	0.43
1:C:47:LYS:HG3	1:C:418:GLU:OE2	2.19	0.43
1:A:59:LEU:HD21	1:A:107:LEU:HD21	2.01	0.43
1:C:149:GLY:O	1:C:170:ALA:HB3	2.17	0.43
1:A:22:LEU:CD1	1:A:22:LEU:N	2.81	0.43
2:D:203:LEU:CD1	2:D:209:ILE:HD11	2.47	0.43
2:B:85:ASN:H	2:B:85:ASN:HD22	1.65	0.43
1:A:175:ALA:CB	1:A:188:THR:HG22	2.49	0.43
2:D:170:PRO:HG3	2:D:243:GLU:HB2	2.01	0.43
2:B:132:GLN:HB3	2:B:293:ASN:HD21	1.83	0.43
1:A:285:GLU:N	1:A:285:GLU:OE1	2.51	0.43
1:A:59:LEU:HD12	1:A:60:GLN:N	2.33	0.43
1:C:10:PRO:HD2	1:C:290:PHE:CZ	2.53	0.43
2:D:272:LEU:HB2	2:D:289:VAL:HG21	2.00	0.43
1:C:175:ALA:HB1	1:C:188:THR:HG22	2.01	0.43
2:D:178:THR:O	2:D:182:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ALA:HA	1:A:401:PHE:HA	2.00	0.43
1:A:309:TYR:CE2	1:A:311:GLU:HA	2.54	0.43
1:A:326:VAL:HG21	1:A:389:LEU:HD21	2.00	0.43
2:D:197:ALA:HB2	2:D:224:TRP:CE3	2.53	0.43
1:A:252:TYR:O	1:A:275:LEU:HD12	2.19	0.43
2:D:169:SER:O	2:D:217:THR:HG22	2.19	0.43
1:A:26:ARG:HB3	1:A:82:ASP:O	2.18	0.43
1:A:247:LEU:HB3	1:A:255:ALA:HB3	2.00	0.42
1:C:189:LEU:HG	1:C:223:LEU:HD13	2.01	0.42
1:C:14:MET:HB3	1:C:343:LEU:HD23	2.01	0.42
2:B:163:PRO:HD3	2:B:209:ILE:HG22	1.99	0.42
1:A:371:ASN:HD21	1:A:385:PRO:HB3	1.84	0.42
1:C:278:LYS:H	1:C:281:GLU:HB2	1.84	0.42
2:D:162:TYR:O	2:D:164:GLN:HG3	2.19	0.42
1:A:26:ARG:HB2	1:A:80:ILE:HG21	2.01	0.42
2:D:239:PHE:CG	2:D:264:LEU:HD11	2.54	0.42
2:D:103:LEU:C	2:D:103:LEU:HD12	2.39	0.42
1:C:363:MET:HB2	1:C:392:LEU:HB3	2.02	0.42
2:B:110:MET:SD	2:B:185:MET:CE	3.07	0.42
1:A:252:TYR:CE2	1:A:278:LYS:HG2	2.55	0.42
1:C:252:TYR:CE2	1:C:278:LYS:HG2	2.54	0.42
1:C:252:TYR:O	1:C:275:LEU:HD12	2.19	0.42
2:B:241:LEU:CD2	2:B:288:VAL:HG11	2.49	0.42
2:D:239:PHE:CD1	2:D:264:LEU:HD11	2.54	0.42
2:D:121:ASN:C	2:D:124:PRO:HD2	2.39	0.42
2:D:168:LEU:CD1	2:D:260:ILE:HD12	2.50	0.42
1:C:309:TYR:CZ	1:C:311:GLU:HA	2.55	0.42
1:A:143:LYS:O	1:A:145:LEU:HG	2.19	0.42
1:A:35:PRO:HD2	1:A:394:THR:HB	2.00	0.42
1:C:354:THR:N	1:C:358:ASP:O	2.41	0.42
2:D:91:VAL:HG12	2:D:93:SER:O	2.20	0.42
1:A:24:LYS:NZ	1:A:78:ASN:HA	2.32	0.42
2:B:197:ALA:HB2	2:B:224:TRP:CE3	2.55	0.42
1:C:375:ILE:HG12	1:C:402:TYR:CE2	2.55	0.42
1:A:324:THR:O	1:A:350:GLU:HA	2.19	0.42
2:D:153:LEU:HD11	2:D:185:MET:HB3	2.03	0.41
2:B:162:TYR:O	2:B:164:GLN:HG3	2.21	0.41
2:D:236:ILE:HG23	2:D:238:VAL:O	2.20	0.41
2:B:121:ASN:C	2:B:124:PRO:HD2	2.41	0.41
2:D:70:LEU:HD21	3:D:480:ADP:C8	2.55	0.41
1:A:131:GLU:C	1:A:133:LYS:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ILE:HG12	1:A:402:TYR:CE2	2.55	0.41
1:A:278:LYS:H	1:A:281:GLU:HB2	1.85	0.41
2:B:77:VAL:CG1	2:B:295:ILE:HG23	2.50	0.41
1:A:244:LEU:HD21	1:A:303:HIS:HB2	2.02	0.41
1:C:100:LEU:CD2	1:C:104:ASN:ND2	2.84	0.41
2:D:157:GLU:OE2	2:D:159:ALA:HB3	2.21	0.41
1:C:285:GLU:OE1	1:C:285:GLU:N	2.54	0.41
1:A:18:GLN:HG2	1:A:404:ILE:HB	2.03	0.41
2:D:145:THR:HG23	2:D:148:PHE:CZ	2.55	0.41
1:A:138:PRO:HG2	1:A:141:TYR:CE2	2.55	0.41
2:D:73:ASN:OD1	2:D:297:LEU:HD11	2.20	0.41
1:C:315:LEU:HD12	1:C:315:LEU:C	2.41	0.41
2:D:238:VAL:HG12	2:D:239:PHE:N	2.35	0.41
2:D:135:ILE:CD1	2:D:285:ALA:HB1	2.49	0.41
2:B:141:GLY:HA2	3:B:480:ADP:C5'	2.47	0.41
1:C:70:GLN:CG	1:C:402:TYR:OH	2.68	0.41
2:D:233:PRO:C	2:D:235:LYS:H	2.23	0.41
1:C:247:LEU:HB3	1:C:255:ALA:HB3	2.03	0.41
2:B:220:THR:O	2:B:224:TRP:CD1	2.74	0.41
2:B:85:ASN:N	2:B:85:ASN:HD22	2.19	0.41
1:C:371:ASN:O	1:C:414:ILE:HD12	2.20	0.41
1:C:169:LEU:HD12	1:C:173:SER:OG	2.21	0.40
2:D:110:MET:SD	2:D:185:MET:HE3	2.62	0.40
1:C:367:VAL:HG11	1:C:369:TYR:CZ	2.56	0.40
2:B:103:LEU:C	2:B:103:LEU:HD12	2.39	0.40
1:C:68:LEU:CD2	1:C:388:VAL:HG11	2.50	0.40
2:D:126:MET:HG2	2:D:271:LEU:HD22	2.02	0.40
1:C:59:LEU:HD12	1:C:60:GLN:N	2.36	0.40
1:A:20:ARG:CZ	1:A:377:ILE:HD13	2.52	0.40
1:C:211:LYS:HZ2	1:C:217:VAL:HG21	1.87	0.40
1:A:80:ILE:HG22	1:A:81:VAL:N	2.37	0.40
1:C:139:PHE:CZ	1:C:426:ARG:NH2	2.90	0.40
1:C:355:ASP:HA	2:D:287:LYS:NZ	2.36	0.40
2:B:247:MET:HG3	2:B:253:HIS:HB3	2.03	0.40
2:D:220:THR:O	2:D:224:TRP:CD1	2.75	0.40
1:A:371:ASN:ND2	1:A:385:PRO:HB3	2.37	0.40
2:B:170:PRO:HG3	2:B:243:GLU:HB2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	418/450 (93%)	371 (89%)	40 (10%)	7 (2%)	11	52
1	C	418/450 (93%)	372 (89%)	38 (9%)	8 (2%)	10	50
2	B	227/479 (47%)	206 (91%)	18 (8%)	3 (1%)	15	59
2	D	227/479 (47%)	205 (90%)	19 (8%)	3 (1%)	15	59
All	All	1290/1858 (69%)	1154 (90%)	115 (9%)	21 (2%)	12	54

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	132	ALA
1	A	264	THR
1	A	423	GLU
2	B	187	LYS
1	C	264	THR
1	C	423	GLU
2	D	187	LYS
1	C	104	ASN
1	C	132	ALA
1	C	147	ASP
1	C	238	ASP
1	A	147	ASP
2	B	227	LYS
2	B	234	LYS
2	D	227	LYS
2	D	234	LYS
1	A	293	PRO
1	C	293	PRO
1	C	35	PRO
1	A	35	PRO

### 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	372/397 (94%)	350 (94%)	22 (6%)	24	65
1	C	372/397 (94%)	351 (94%)	21 (6%)	26	68
2	B	203/418 (49%)	192 (95%)	11 (5%)	27	68
2	D	203/418 (49%)	192 (95%)	11 (5%)	27	68
All	All	1150/1630 (71%)	1085 (94%)	65 (6%)	25	67

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	41	LEU
1	A	44	VAL
1	A	75	ASP
1	A	85	GLN
1	A	104	ASN
1	A	114	SER
1	A	126	ARG
1	A	143	LYS
1	A	168	CYS
1	A	212	GLN
1	A	324	THR
1	A	334	ASP
1	A	355	ASP
1	A	363	MET
1	A	373	VAL
1	A	378	SER
1	A	413	LEU
1	A	416	THR
1	A	420	LEU
1	A	421	SER
1	A	427	GLN
2	B	85	ASN
2	B	89	TYR

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Mol	Chain	Res	Type
2	B	102	GLN
2	B	103	LEU
2	B	145	THR
2	B	166	LEU
2	B	173	GLU
2	B	199	ARG
2	B	209	ILE
2	B	253	HIS
2	B	276	THR
1	C	40	SER
1	C	44	VAL
1	C	75	ASP
1	C	85	GLN
1	C	104	ASN
1	C	114	SER
1	C	126	ARG
1	C	127	THR
1	C	143	LYS
1	C	168	CYS
1	C	182	THR
1	C	324	THR
1	C	334	ASP
1	C	355	ASP
1	C	363	MET
1	C	373	VAL
1	C	413	LEU
1	C	416	THR
1	C	420	LEU
1	C	421	SER
1	C	427	GLN
2	D	85	ASN
2	D	89	TYR
2	D	102	GLN
2	D	103	LEU
2	D	145	THR
2	D	166	LEU
2	D	173	GLU
2	D	199	ARG
2	D	209	ILE
2	D	253	HIS
2	D	276	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	71	ASN
1	A	78	ASN
1	A	212	GLN
1	A	218	GLN
1	A	427	GLN
2	B	81	GLN
2	B	85	ASN
2	B	286	GLN
1	C	60	GLN
1	C	71	ASN
1	C	78	ASN
1	C	212	GLN
1	C	218	GLN
1	C	427	GLN
2	D	81	GLN
2	D	85	ASN
2	D	286	GLN

### 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](#)

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	ADP	B	480	-	22,29,29	0.83	1 (4%)	27,45,45	2.38	2 (7%)
3	ADP	D	480	-	22,29,29	0.84	1 (4%)	27,45,45	2.50	4 (14%)

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	ADP	B	480	-	-	0/12/32/32	0/3/3/3
3	ADP	D	480	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	480	ADP	O4'-C1'	2.51	1.44	1.41
3	D	480	ADP	O4'-C1'	2.55	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	480	ADP	N3-C2-N1	-11.06	120.43	128.89
3	B	480	ADP	N3-C2-N1	-10.60	120.78	128.89
3	D	480	ADP	PA-O3A-PB	-3.19	121.95	132.67
3	B	480	ADP	PA-O3A-PB	-3.02	122.55	132.67
3	D	480	ADP	O3A-PA-O5'	-2.30	96.82	102.94
3	D	480	ADP	O3B-PB-O2B	2.18	115.68	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	480	ADP	4	0
3	D	480	ADP	3	0



## 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	420/450 (93%)	0.78	39 (9%) 11 6	83, 86, 88, 91	0
1	C	420/450 (93%)	0.73	36 (8%) 13 7	83, 86, 88, 91	0
2	B	229/479 (47%)	0.64	15 (6%) 22 12	84, 86, 88, 89	0
2	D	229/479 (47%)	0.64	10 (4%) 38 24	84, 86, 88, 89	0
All	All	1298/1858 (69%)	0.71	100 (7%) 16 9	83, 86, 88, 91	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ALA	7.9
1	A	279	LYS	7.0
1	C	279	LYS	5.9
1	C	274	ALA	5.9
1	C	280	GLU	3.9
2	D	297	LEU	3.8
1	A	280	GLU	3.8
1	A	316	VAL	3.5
1	C	275	LEU	3.4
1	C	239	HIS	3.3
1	A	308	SER	3.2
1	A	275	LEU	3.2
1	C	68	LEU	3.1
1	A	239	HIS	3.1
1	A	276	LEU	3.1
1	A	318	ALA	3.1
1	C	287	PHE	3.0
1	A	68	LEU	3.0
1	A	287	PHE	3.0
1	A	67	LEU	3.0
1	A	238	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	142	THR	2.9
2	B	244	ALA	2.9
2	B	233	PRO	2.9
1	C	69	ILE	2.8
1	A	282	LYS	2.8
2	B	277	PHE	2.8
1	A	265	LEU	2.8
1	C	62	PHE	2.8
1	C	379	ASP	2.7
1	A	69	ILE	2.7
1	C	67	LEU	2.7
2	B	73	ASN	2.7
1	C	282	LYS	2.6
1	A	254	PHE	2.6
1	C	293	PRO	2.6
1	C	265	LEU	2.6
1	A	307	LEU	2.5
1	A	228	VAL	2.5
1	A	317	LEU	2.5
1	C	319	ALA	2.5
1	A	52	PHE	2.5
2	D	233	PRO	2.5
1	C	273	MET	2.5
1	A	290	PHE	2.4
1	C	305	TYR	2.4
1	C	276	LEU	2.4
2	D	277	PHE	2.4
1	C	254	PHE	2.4
1	C	316	VAL	2.4
2	B	118	ILE	2.4
2	D	89	TYR	2.4
1	C	107	LEU	2.4
2	D	118	ILE	2.4
1	A	273	MET	2.3
1	A	298	CYS	2.3
1	A	404	ILE	2.3
1	C	34	LEU	2.3
1	C	283	HIS	2.3
1	A	403	MET	2.3
1	A	319	ALA	2.3
1	C	271	VAL	2.3
2	D	77	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	209	ILE	2.3
2	B	297	LEU	2.3
1	C	318	ALA	2.3
2	D	71	VAL	2.3
1	C	52	PHE	2.3
1	C	398	LEU	2.2
1	A	216	VAL	2.2
1	A	266	GLU	2.2
1	A	247	LEU	2.2
1	A	106	THR	2.2
1	C	295	TYR	2.2
2	B	72	ASP	2.2
1	A	229	ILE	2.2
1	A	392	LEU	2.2
1	C	317	LEU	2.2
1	C	238	ASP	2.2
1	C	392	LEU	2.2
2	B	231	ILE	2.1
1	C	420	LEU	2.1
1	C	326	VAL	2.1
1	A	62	PHE	2.1
1	C	403	MET	2.1
1	A	107	LEU	2.1
1	A	256	ILE	2.1
1	C	248	TRP	2.1
2	B	260	ILE	2.1
1	A	329	LEU	2.1
1	C	143	LYS	2.1
2	D	172	TYR	2.1
1	A	285	GLU	2.1
2	B	126	MET	2.1
2	B	209	ILE	2.1
2	B	166	LEU	2.1
2	B	70	LEU	2.0
2	B	71	VAL	2.0
1	A	300	GLU	2.0
2	B	168	LEU	2.0

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

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	ADP	B	480	27/27	0.92	0.17	-1.50	85,89,89,90	0
3	ADP	D	480	27/27	0.92	0.17	-1.53	84,91,92,92	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.