Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 03:09 PM EDT

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)

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

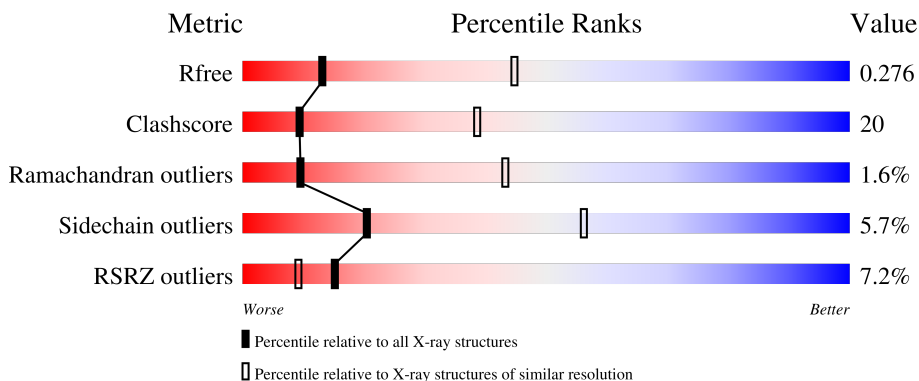|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	Percentile Ranks	Value
Rfree		0.276
Clashscore		20
Ramachandran outliers		1.6%
Sidechain outliers		5.7%
RSRZ outliers		7.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	8% 61% 29% • 7%
1	C	450	8% 60% 31% • 7%
2	B	479	2% 29% 18% • 52%
2	D	479	2% 28% 19% • 52%

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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 (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Nuclear pore complex protein Nup214

Chain A:

- Molecule 1: Nuclear pore complex protein Nup214

Chain C:

S393 T394 L398 C399 P400 F401 Y402 M403 N407 V410 L413 I414 K415 T416 P417 E418 R419 L420 S421 L422 E423 R426 Q427 P428 LYS SER PRO GLY SER THR PRO THR PRO THR SER SER GLN ALA PRO GLN LYS LEU ASP ALA SER

• Molecule 2: ATP-dependent RNA helicase DDX19B

Chain B:

2%

29%　　　　18%　•　　　52%

MET ALA THR ASP SER TRP ALA LEU ALA VAL ASP GLU GLN GLN GLU ALA ALA ALA GLU SER LEU SER ASN LEU HIS LEU LYS GLU GLU LYS ILE LYS PRO ASP THR ASN GLY VAL ALA VAL VAL LYS THR ASN ALA ASN ALA GLU LYS THR ASP GLU GLU GLU LYS GLU ASP ARG ALA ALA GLN SER

LEU LEU ASN LYS LEU ILE ARG SER ASN L70 V71 D72 N73 T74 N75 Q76 V77 L80 N85 Y89 S90 V91 K92 S93 F94 E95 E96 L97 R98 Q102 L103 M110 I118 N121 A122 L123 P124 L127 P130 P131 Q132 N133 L134 I135 G141 T142 T145 F148

V149 L150 A151 M152 L153 V156 E157 P158 A159 Y162 P163 Q164 C165 L166 C167 L168 S169 P170 T171 Y172 E173 L174 Q184 M185 G186 K187 L192 A195 Y196 A197 V198 R199 L203 I209 S210 E211 Q212 I213 V214 T220 V221 L222 D223 W224 K227 I231 D232 P233 K234 K235

I236 F239 V240 L241 D242 E243 A244 M247 H253 I260 L264 C268 Q269 M270 L271 L272 F273 T276 F277 K283 F284 A285 Q286 K287 V288 V289 N293 V294 I295 K296 L297 K298 ARG GLU GLU GLU THR LEU ASP THR ILE LYS GLN TYR TYR VAL LEU CYS SER SER ARG

ASP GLU LYS PHE GLN ALA LEU CYS ASN LEU TYR GLY ALA ILE THR ILE ALA GLN ALA MET ILE PHE CYS HIS THR ARG LYS THR ALA SER TRP LEU ALA ALA GLU LEU SER LYS GLU GLY HIS GLN VAL ALA LEU LEU SER GLU MET VAL GLU GLN ARG ALA ALA VAL LEU CYS SER SER ARG

ARG PHE ARG GLU GLY LYS GLU LYS VAL LEU VAL LEU THR THR ASN VAL CYS ALA ARG GLY ILE ASP VAL GLN GLN VAL SER VAL VAL ILE ASN PHE ASP LEU PRO VAL ASP ASP SER LYS ASP SER GLY GLY HIS GLN VAL ALA LEU LEU SER GLU MET VAL GLU GLN ARG ALA ALA VAL LEU CYS SER SER ARG

LEU ALA VAL ASN MET VAL ASP SER LYS HIS SER MET ASN ILE LEU ASN ARG ILE GLU GLU HIS PHE ASN LYS ILE GLU GLU ARG LEU LEU GLU ILE GLU ILE ALA ASN
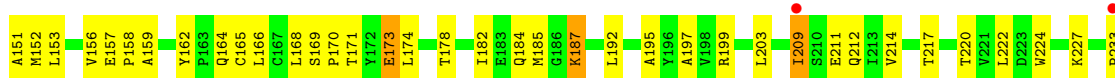
• Molecule 2: ATP-dependent RNA helicase DDX19B

Chain D:

2%

28%　　　　19%　•　　　52%

MET ALA THR ASP SER TRP ALA LEU ALA VAL ASP GLU GLN GLN GLU ALA ALA ALA GLU SER LEU SER ASN LEU HIS LEU LYS GLU GLU LYS ILE LYS PRO ASP THR ASN GLY VAL ALA VAL VAL LYS THR ASN ALA ASN ALA GLU LYS THR ASP GLU GLU GLU LYS GLU ASP ARG ALA ALA GLN SER

LEU LEU ASN LYS LEU ILE ARG SER ASN L70 V71 D72 N73 T74 N75 Q76 V77 L80 N85 Y89 S90 V91 K92 S93 F94 E95 E96 L97 R98 Q102 L103 M110 I118 N121 A122 L123 P124 M126 L127 I135 S138 T142 G143 K144 T145 F148 V149 L150

A151 M152 L153 V156 E157 P158 A159 Y162 P163 Q164 C165 L166 C167 L168 S169 P170 T171 Y172 E173 L174 T178 I182 E183 Q184 M185 G186 K187 L192 A195 Y196 A197 V198 R199 L203 I209 S210 E211 Q212 I213 V214 T217 T220 V221 L222 D223 W224 K227 P233

K234 K235 I236 K237 V238 F239 V240 L241 D242 E243 A244 H253 I260 L264 C268 Q269 M270 L271 L272 F273 T276 F277 K283 F284 A285 Q286 K287 V288 V289 V294 I295 K296 L297 K298 ARG GLU GLU GLU THR LEU ASP THR ILE LYS GLN TYR TYR VAL LEU CYS SER SER ARG

ASP GLU LYS PHE GLN ALA LEU CYS ASN LEU TYR GLY ALA ILE THR ILE ALA GLN ALA MET ILE PHE CYS HIS THR ARG LYS THR ALA SER TRP LEU ALA ALA GLU LEU SER LYS GLU GLY MET VAL GLU GLN ARG ALA ALA VAL LEU CYS SER SER ARG

ARG PHE ARG GLU GLY LYS GLU LYS VAL LEU VAL LEU THR THR ASN VAL CYS ALA ARG GLY ILE ASP VAL GLN GLN VAL SER VAL VAL ILE ASN PHE ASP LEU PRO VAL ASP ASP SER LYS ASP SER GLY GLY HIS GLN VAL ALA LEU LEU SER GLU MET VAL GLU GLN ARG ALA ALA VAL LEU CYS SER SER ARG

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, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	92.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 84.2	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10216	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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
1:A:149:GLY:O	1:A:170:ALA:HB3	1.97	0.64
2:B:91:VAL:HG23	2:B:124:PRO:HG3	1.80	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
1:A:20:ARG:NH1	1:A:377:ILE:HD12	2.14	0.63
2:B:168:LEU:HD11	2:B:260:ILE:HD12	1.80	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:HD12	2:B:103:LEU:O	2.01	0.59
1:A:21:ALA:HB2	1:A:401:PHE:CD2	2.38	0.59
2:D:171:THR:OG1	2:D:174:LEU:HD13	2.02	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
1:A:22:LEU:N	1:A:22:LEU:HD12	2.18	0.58
2:D:184:GLN:O	2:D:187:LYS:HB2	2.03	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:23:LYS:HZ1	1:A:75:ASP:HB3	1.69	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
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:A:153:ILE:HG23	1:A:170:ALA:N	2.19	0.57
1:C:21:ALA:HB2	1:C:401:PHE:CE2	2.39	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
1:C:61:ILE:HD12	1:C:61:ILE:N	2.20	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
2:D:152:MET:HE2	2:D:165:CYS:HB3	1.86	0.56
1:A:9:ILE:N	1:A:10:PRO:CD	2.69	0.56
2:D:244:ALA:HB2	2:D:272:LEU:HD21	1.88	0.56
2:B:244:ALA:HB2	2:B:272:LEU:HD21	1.88	0.55
2:D:95:GLU:OE1	2:D:95:GLU:N	2.32	0.55
2:D:152:MET:O	2:D:156:VAL:HG23	2.05	0.55
1:A:64:THR:HG21	1:A:368:ASP:OD1	2.05	0.55
1:A:427:GLN:HE21	1:A:427:GLN:N	2.04	0.55
2:B:268:CYS:SG	2:B:270:MET:HE1	2.46	0.55
1:C:138:PRO:HG2	1:C:141:TYR:CZ	2.42	0.55
1:A:61:ILE:HD12	1:A:61:ILE:N	2.20	0.55
2:B:118:ILE:HB	2:B:142:THR:HG22	1.89	0.55
2:B:184:GLN:O	2:B:187:LYS:HB2	2.06	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
1:A:103:ASP:OD1	1:A:104:ASN:N	2.42	0.52
2:D:270:MET:HB2	2:D:289:VAL:HG13	1.91	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
2:B:130:PRO:HD3	1:C:187:ALA:HB2	1.92	0.52
1:C:153:ILE:CG2	1:C:170:ALA:HA	2.40	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:N	1:C:22:LEU:HD12	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
2:B:80:LEU:HB2	2:B:294:VAL:HB	1.93	0.51
1:C:187:ALA:HB1	1:C:223:LEU:HD12	1.93	0.51
1:C:208:ALA:HB2	1:C:248:TRP:CZ3	2.46	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:A:138:PRO:HG2	1:A:141:TYR:CZ	2.46	0.51
1:C:10:PRO:HD2	1:C:290:PHE:CE2	2.46	0.51
1:A:187:ALA:HB1	1:A:223:LEU:HD12	1.92	0.50
2:B:156:VAL:HG22	2:B:165:CYS:SG	2.51	0.50
1:C:363:MET:HE3	1:C:363:MET:HA	1.93	0.50
2:D:268:CYS:SG	2:D:270:MET:HE1	2.51	0.50
1:A:108:SER:OG	1:A:108:SER:O	2.12	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
2:D:91:VAL:HG21	2:D:97:LEU:HD21	1.92	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
1:C:326:VAL:HB	1:C:349:ALA:HB3	1.92	0.50
2:D:80:LEU:HB2	2:D:294:VAL:HB	1.93	0.50
1:A:100:LEU:CD2	1:A:104:ASN:ND2	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:MET:SD	1:C:394:THR:HG22	2.52	0.50
2:D:91:VAL:CG1	2:D:96:GLU:OE1	2.60	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
2:B:134:LEU:HD12	2:B:293:ASN:O	2.12	0.49
1:C:100:LEU:HD23	1:C:104:ASN:ND2	2.27	0.49
1:A:211:LYS:NZ	1:A:217:VAL:HG21	2.27	0.49
1:C:61:ILE:N	1:C:61:ILE:CD1	2.76	0.49
1:C:351:LEU:HD13	1:C:361:LEU:HA	1.93	0.49
2:D:284:PHE:CE1	2:D:288:VAL:HG21	2.48	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:B:152:MET:CE	2:B:165:CYS:HB3	2.42	0.49
2:D:173:GLU:O	2:D:174:LEU:HD12	2.13	0.49
1:A:9:ILE:N	1:A:10:PRO:HD2	2.27	0.48
2:B:70:LEU:HD11	3:B:480:ADP:C5	2.48	0.48
2:B:297:LEU:HD12	2:B:298:LYS:N	2.29	0.48
2:B:209:ILE:HG23	2:B:211:GLU:OE1	2.13	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
1:A:59:LEU:HD21	1:A:107:LEU:CD2	2.43	0.48
1:A:174:ILE:CG2	1:A:189:LEU:HB2	2.43	0.48
2:D:268:CYS:O	2:D:270:MET:HE3	2.13	0.48
1:A:61:ILE:N	1:A:61:ILE:CD1	2.76	0.48
1:A:326:VAL:HB	1:A:349:ALA:HB3	1.95	0.48
2:B:152:MET:HE2	2:B:165:CYS: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:20:ARG:NH1	1:C:377:ILE:HD12	2.28	0.48
1:C:309:TYR:CE2	1:C:311:GLU:HA	2.49	0.48
1:A:263:GLY:O	1:A:265:LEU:N	2.47	0.48
1:A:363:MET:HE3	1:A:363:MET:HA	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:C:24:LYS:HZ1	1:C:78:ASN:HA	1.79	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)
2:D:239:PHE:HB3	2:D:270:MET:HE2	1.95	0.47
2:B:272:LEU:HB2	2:B:289:VAL:HG21	1.97	0.47
2:B:283:LYS:HA	2:B:286:GLN:HE21	1.79	0.47
2:D:123:LEU:HB3	2:D:127:LEU:HD12	1.94	0.47
2:D:241:LEU:HD21	2:D:288:VAL:HG11	1.96	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
1:A:363:MET:SD	1:A:394:THR:HG22	2.54	0.47
2:D:241:LEU:CD2	2:D:288:VAL:HG11	2.45	0.47
2:D:283:LYS:HA	2:D:286:GLN:HE21	1.80	0.47
1:A:354:THR:N	1:A:358:ASP:O	2.39	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
2:B:70:LEU:HD21	3:B:480:ADP:C8	2.50	0.47
1:C:59:LEU:HD12	1:C:60:GLN:H	1.79	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
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:17:PHE:CE1	1:A:328:ILE:HD11	2.50	0.46
2:B:135:ILE:CD1	2:B:285:ALA:HB1	2.45	0.46
1:C:59:LEU:HD21	1:C:107:LEU:CD2	2.45	0.46
2:D:297:LEU:HD12	2:D:298:LYS:N	2.30	0.46
1:C:175:ALA:CB	1:C:188:THR:HG22	2.46	0.46
2:D:85:ASN:N	2:D:85:ASN:ND2	2.63	0.46
1:A:124:ASP:OD2	1:A:126:ARG:NH1	2.48	0.46
1:A:200:TRP:CH2	1:A:207:LEU:HD22	2.50	0.46
1:A:209:VAL:HG23	1:A:209:VAL:O	2.14	0.46
1:C:24:LYS:CE	1:C:78:ASN:HA	2.46	0.46
2:D:148:PHE:O	2:D:151:ALA:HB3	2.16	0.46
2:D:222:LEU:O	2:D:222:LEU:HD12	2.16	0.46
1:A:156:LYS:HD2	1:A:198:VAL:HG12	1.98	0.46
1:C:200:TRP:CH2	1:C:207:LEU:HD22	2.50	0.46
1:C:244:LEU:HD21	1:C:303:HIS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:VAL:HG22	1:C:403:MET:HE2	1.98	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
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: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
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
2:B:123:LEU:N	2:B:124:PRO:CD	2.79	0.46
2:B:268:CYS:SG	2:B:270:MET:HE2	2.55	0.46
1:A:291:MET:O	1:A:292:GLU:C	2.54	0.45
2:B:75:ASN:HB3	2:B:298:LYS:HB2	1.98	0.45
1:C:40:SER:O	1:C:41:LEU:HD23	2.16	0.45
1:C:138:PRO:HG2	1:C:141:TYR:CE2	2.51	0.45
1:C:375:ILE:HG12	1:C:402:TYR:CD2	2.50	0.45
1:A:104:ASN:HD22	1:A:104:ASN:HA	1.53	0.45
1:C:112:MET:CE	1:C:118:SER:HB3	2.45	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:B:192:LEU:HA	2:B:212:GLN:NE2	2.32	0.45
1:C:23:LYS:HZ2	1:C:23:LYS:HG2	1.70	0.45
1:C:75:ASP:OD1	1:C:75:ASP:N	2.48	0.45
2:D:121:ASN:O	2:D:124:PRO:HD2	2.17	0.45
2:D:85:ASN:H	2:D:85:ASN:HD22	1.65	0.45
1:A:75:ASP:N	1:A:75:ASP:OD1	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: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
1:C:361:LEU:O	1:C:393:SER:HA	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:106:THR:O	1:C:106:THR:HG22	2.18	0.44
1:C:212:GLN:NE2	1:C:242:ARG:HD2	2.31	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
1:C:157:TRP:HA	1:C:165:VAL:HG23	2.00	0.44
2:D:70:LEU:HD11	3:D:480:ADP:C6	2.53	0.44
2:D:123:LEU:N	2:D:124:PRO:CD	2.80	0.44
1:C:427:GLN:HE21	1:C:427:GLN:N	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
1:A:10:PRO:HD2	1:A:290:PHE:CZ	2.53	0.43
1:C:26:ARG:HB3	1:C:82:ASP:O	2.18	0.43
2:D:75:ASN:HB3	2:D:298:LYS:HB2	1.98	0.43
2:D:150:LEU:O	2:D:151:ALA:C	2.56	0.43
1:A:175:ALA:HB1	1:A:188:THR:HG22	2.00	0.43
2:B:153:LEU:HD11	2:B:185:MET:HB3	2.00	0.43
2:B:222:LEU:HD12	2:B:222:LEU:O	2.17	0.43
1:C:24:LYS:HZ3	1:C:78:ASN:HD22	1.65	0.43
1:A:312:GLU:H	1:A:312:GLU:CD	2.21	0.43
2:B:203:LEU:CD1	2:B:209:ILE:HD11	2.48	0.43
1:C:47:LYS:HG3	1:C:418:GLU:OE2	2.19	0.43
1:C:326:VAL:HG21	1:C:389:LEU:HD21	2.00	0.43
1:A:22:LEU:N	1:A:22:LEU:CD1	2.81	0.43
1:A:59:LEU:HD21	1:A:107:LEU:HD21	2.01	0.43
1:A:175:ALA:CB	1:A:188:THR:HG22	2.49	0.43
2:B:85:ASN:H	2:B:85:ASN:HD22	1.65	0.43
1:C:149:GLY:O	1:C:170:ALA:HB3	2.17	0.43
2:D:203:LEU:CD1	2:D:209:ILE:HD11	2.47	0.43
2:D:170:PRO:HG3	2:D:243:GLU:HB2	2.01	0.43
1:A:285:GLU:N	1:A:285:GLU:OE1	2.51	0.43
2:B:132:GLN:HB3	2:B:293:ASN:HD21	1.83	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
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
2:D:272:LEU:HB2	2:D:289:VAL:HG21	2.00	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
1:A:26:ARG:HB3	1:A:82:ASP:O	2.18	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
2:D:197:ALA:HB2	2:D:224:TRP:CE3	2.53	0.43
1:A:247:LEU:HB3	1:A:255:ALA:HB3	2.00	0.42
1:C:14:MET:HB3	1:C:343:LEU:HD23	2.01	0.42
1:C:189:LEU:HG	1:C:223:LEU:HD13	2.01	0.42
1:A:371:ASN:HD21	1:A:385:PRO:HB3	1.84	0.42
2:B:163:PRO:HD3	2:B:209:ILE:HG22	1.99	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
1:A:252:TYR:CE2	1:A:278:LYS:HG2	2.55	0.42
2:B:110:MET:SD	2:B:185:MET:CE	3.07	0.42
1:C:252:TYR:O	1:C:275:LEU:HD12	2.19	0.42
1:C:252:TYR:CE2	1:C:278:LYS:HG2	2.54	0.42
1:C:363:MET:HB2	1:C:392:LEU:HB3	2.02	0.42
2:D:103:LEU:HD12	2:D:103:LEU:C	2.39	0.42
2:D:239:PHE:CG	2:D:264:LEU:HD11	2.54	0.42
1:A:143:LYS:O	1:A:145:LEU:HG	2.19	0.42
2:B:241:LEU:CD2	2:B:288:VAL:HG11	2.49	0.42
1:C:309:TYR:CZ	1:C:311:GLU:HA	2.55	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
2:D:239:PHE:CD1	2:D:264:LEU:HD11	2.54	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
1:A:24:LYS:NZ	1:A:78:ASN:HA	2.32	0.42
1:A:324:THR:O	1:A:350:GLU:HA	2.19	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
2:D:91:VAL:HG12	2:D:93:SER:O	2.20	0.42
2:B:162:TYR:O	2:B:164:GLN:HG3	2.21	0.41
2:D:153:LEU:HD11	2:D:185:MET:HB3	2.03	0.41
1:A:131:GLU:C	1:A:133:LYS:H	2.22	0.41
1:A:244:LEU:HD21	1:A:303:HIS:HB2	2.02	0.41
1:A:278:LYS:H	1:A:281:GLU:HB2	1.85	0.41
1:A:375:ILE:HG12	1:A:402:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:VAL:CG1	2:B:295:ILE:HG23	2.50	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
2:D:236:ILE:HG23	2:D:238:VAL:O	2.20	0.41
1:A:18:GLN:HG2	1:A:404:ILE:HB	2.03	0.41
1:C:100:LEU:CD2	1:C:104:ASN:ND2	2.84	0.41
1:C:285:GLU:N	1:C:285:GLU:OE1	2.54	0.41
2:D:157:GLU:OE2	2:D:159:ALA:HB3	2.21	0.41
1:A:138:PRO:HG2	1:A:141:TYR:CE2	2.55	0.41
1:C:315:LEU:C	1:C:315:LEU:HD12	2.41	0.41
2:D:73:ASN:OD1	2:D:297:LEU:HD11	2.20	0.41
2:D:145:THR:HG23	2:D:148:PHE:CZ	2.55	0.41
2:D:135:ILE:CD1	2:D:285:ALA:HB1	2.49	0.41
2:D:238:VAL:HG12	2:D:239:PHE:N	2.35	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:B:85:ASN:N	2:B:85:ASN:HD22	2.19	0.41
2:B:220:THR:O	2:B:224:TRP:CD1	2.74	0.41
1:C:247:LEU:HB3	1:C:255:ALA:HB3	2.03	0.41
1:C:371:ASN:O	1:C:414:ILE:HD12	2.20	0.41
2:D:233:PRO:C	2:D:235:LYS:H	2.23	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
2:B:103:LEU:HD12	2:B:103:LEU:C	2.39	0.40
1:C:68:LEU:CD2	1:C:388:VAL:HG11	2.50	0.40
1:C:367:VAL:HG11	1:C:369:TYR:CZ	2.56	0.40
2:D:126:MET:HG2	2:D:271:LEU:HD22	2.02	0.40
1:A:20:ARG:CZ	1:A:377:ILE:HD13	2.52	0.40
1:A:80:ILE:HG22	1:A:81:VAL:N	2.37	0.40
2:B:247:MET:HG3	2:B:253:HIS:HB3	2.03	0.40
1:C:59:LEU:HD12	1:C:60:GLN:N	2.36	0.40
1:C:139:PHE:CZ	1:C:426:ARG:NH2	2.90	0.40
1:C:211:LYS:HZ2	1:C:217:VAL:HG21	1.87	0.40
1:C:355:ASP:HA	2:D:287:LYS:NZ	2.36	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
2:D:220:THR:O	2:D:224:TRP:CD1	2.75	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%)	9	42
1	C	418/450 (93%)	372 (89%)	38 (9%)	8 (2%)	8	39
2	B	227/479 (47%)	206 (91%)	18 (8%)	3 (1%)	12	47
2	D	227/479 (47%)	205 (90%)	19 (8%)	3 (1%)	12	47
All	All	1290/1858 (69%)	1154 (90%)	115 (9%)	21 (2%)	9	43

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 (i)

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%)	19	54
1	C	372/397 (94%)	351 (94%)	21 (6%)	21	57
2	B	203/418 (49%)	192 (95%)	11 (5%)	22	58
2	D	203/418 (49%)	192 (95%)	11 (5%)	22	58
All	All	1150/1630 (71%)	1085 (94%)	65 (6%)	20	56

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

Sometimes 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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	B	480	-	24,29,29	0.86	1 (4%)	29,45,45	1.47	3 (10%)
3	ADP	D	480	-	24,29,29	0.85	1 (4%)	29,45,45	1.52	3 (10%)

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	-	-	4/12/32/32	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	D	480	ADP	O4'-C1'	2.40	1.44	1.41
3	B	480	ADP	O4'-C1'	2.36	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	480	ADP	N3-C2-N1	-5.28	120.43	128.68
3	B	480	ADP	N3-C2-N1	-5.05	120.78	128.68
3	D	480	ADP	PA-O3A-PB	-3.17	121.95	132.83
3	B	480	ADP	PA-O3A-PB	-2.99	122.55	132.83
3	B	480	ADP	C3'-C2'-C1'	2.86	105.29	100.98
3	D	480	ADP	O3B-PB-O2B	2.10	115.68	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	480	ADP	C5'-O5'-PA-O1A
3	B	480	ADP	C5'-O5'-PA-O3A
3	B	480	ADP	C4'-C5'-O5'-PA
3	B	480	ADP	C5'-O5'-PA-O2A

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP B 480

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 480

Bond lengths

Bond angles

Torsions

Rings
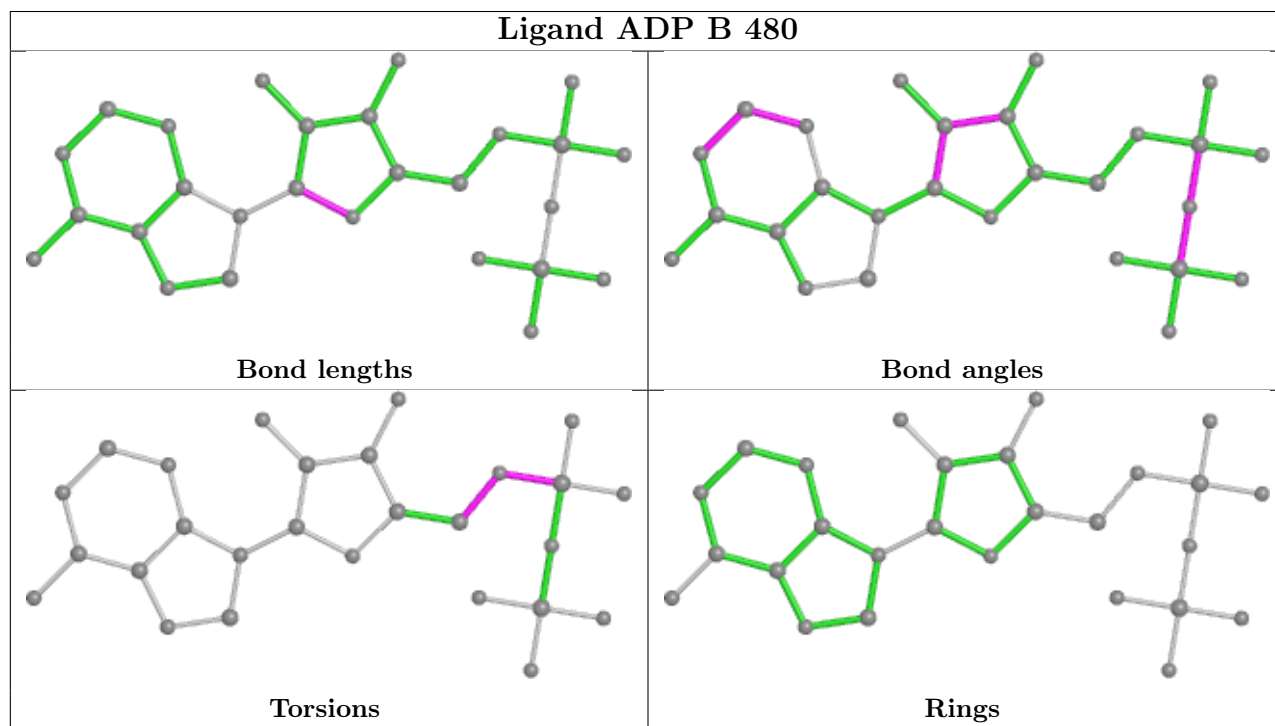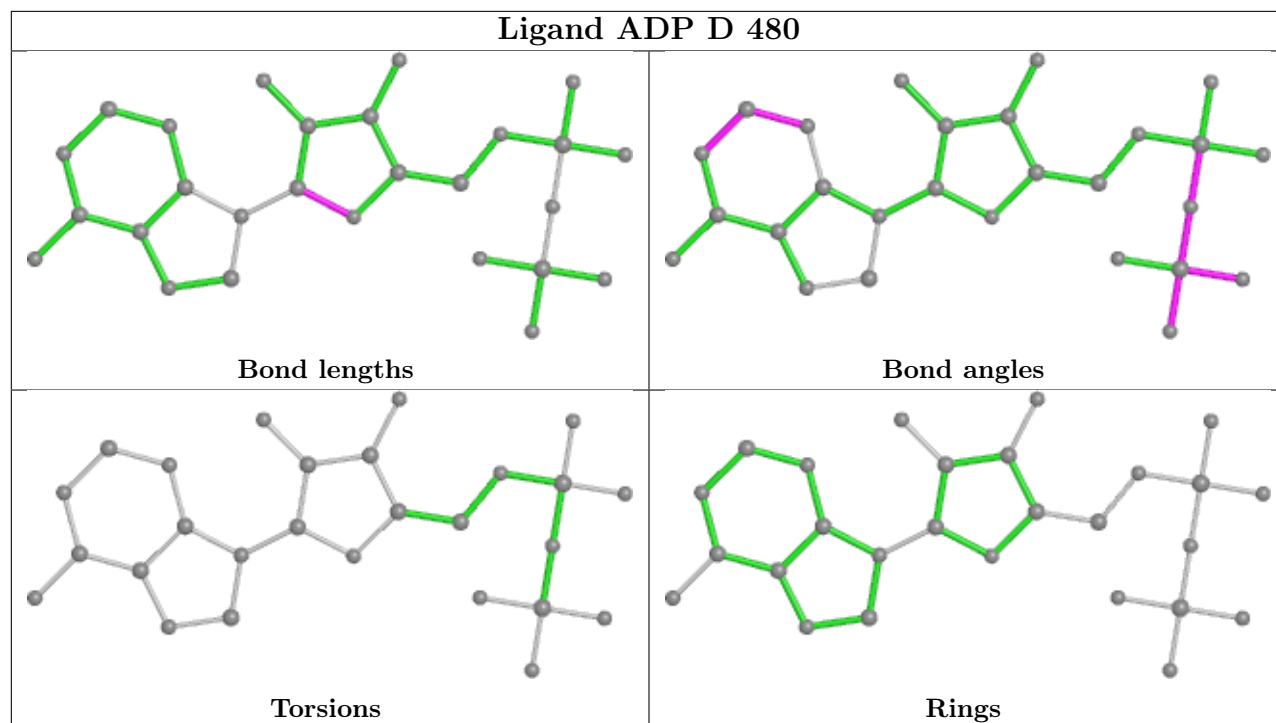
5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	A	420/450 (93%)	0.74	38 (9%)	9	5	83, 86, 88, 90	0
1	C	420/450 (93%)	0.69	36 (8%)	10	5	83, 86, 88, 91	0
2	B	229/479 (47%)	0.60	10 (4%)	34	21	84, 86, 88, 89	0
2	D	229/479 (47%)	0.61	9 (3%)	39	25	84, 86, 88, 89	0
All	All	1298/1858 (69%)	0.67	93 (7%)	15	9	83, 86, 88, 91	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ALA	7.7
1	A	279	LYS	6.8
1	C	279	LYS	5.8
1	C	274	ALA	5.7
1	C	280	GLU	3.8
1	A	280	GLU	3.7
2	D	297	LEU	3.7
1	A	316	VAL	3.4
1	C	275	LEU	3.3
1	C	239	HIS	3.2
1	A	308	SER	3.1
1	A	275	LEU	3.1
1	A	239	HIS	3.0
1	C	68	LEU	3.0
1	A	276	LEU	3.0
1	A	318	ALA	3.0
1	C	287	PHE	2.9
1	A	68	LEU	2.9
1	A	287	PHE	2.9
1	A	67	LEU	2.9
1	A	238	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	244	ALA	2.8
2	D	142	THR	2.8
2	B	233	PRO	2.8
1	C	69	ILE	2.7
2	B	277	PHE	2.7
1	A	282	LYS	2.7
1	A	265	LEU	2.7
1	C	62	PHE	2.7
1	C	379	ASP	2.7
1	A	69	ILE	2.7
2	B	73	ASN	2.6
1	C	67	LEU	2.6
1	C	282	LYS	2.5
1	A	254	PHE	2.5
1	C	293	PRO	2.5
1	C	265	LEU	2.5
1	A	307	LEU	2.4
1	A	228	VAL	2.4
1	C	319	ALA	2.4
1	A	317	LEU	2.4
1	A	52	PHE	2.4
2	D	233	PRO	2.4
1	C	273	MET	2.3
1	A	290	PHE	2.3
1	C	276	LEU	2.3
2	D	277	PHE	2.3
1	C	305	TYR	2.3
2	B	118	ILE	2.3
1	C	254	PHE	2.3
2	D	118	ILE	2.3
1	C	316	VAL	2.3
1	C	107	LEU	2.3
1	A	404	ILE	2.3
1	C	283	HIS	2.3
1	A	298	CYS	2.3
2	D	89	TYR	2.3
1	A	273	MET	2.2
1	C	34	LEU	2.2
2	D	209	ILE	2.2
1	C	271	VAL	2.2
1	A	319	ALA	2.2
2	D	77	VAL	2.2

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

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

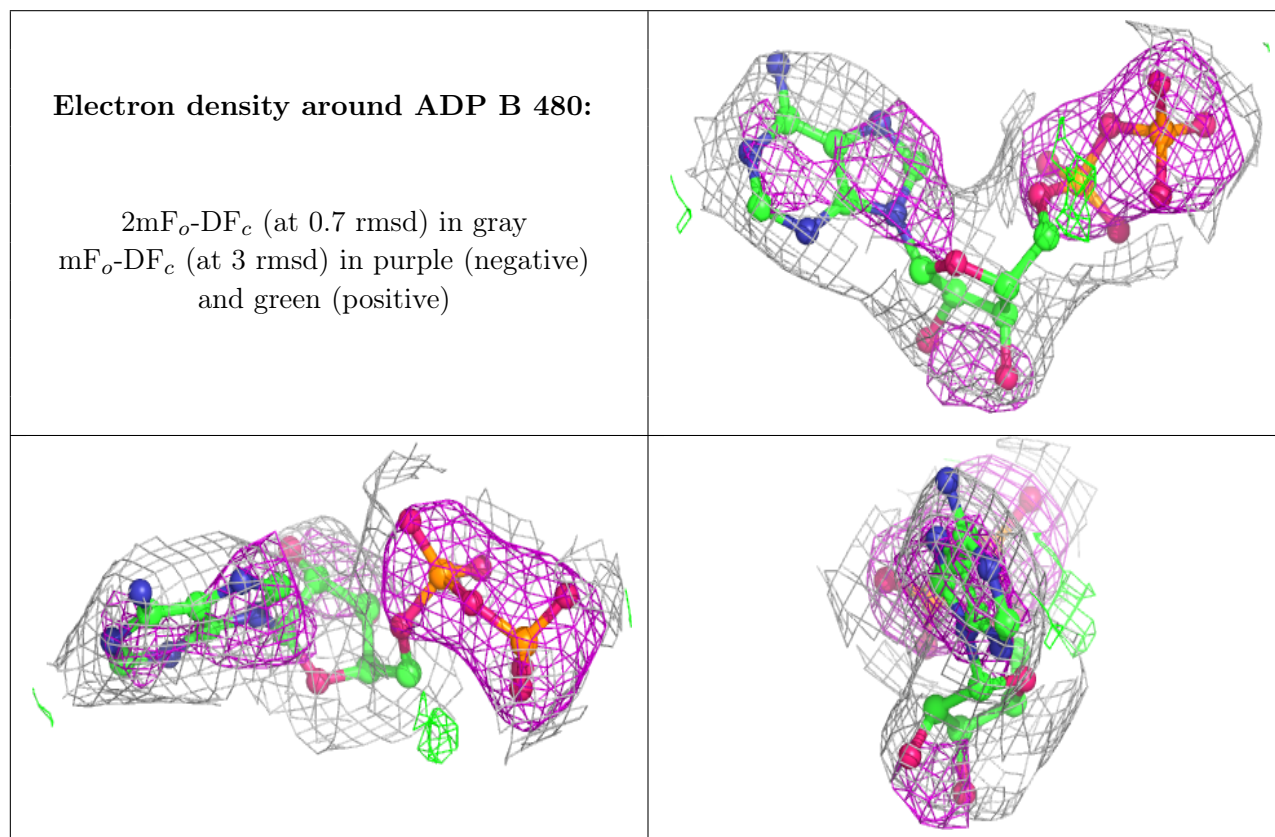There are no non-standard protein/DNA/RNA residues in this entry.

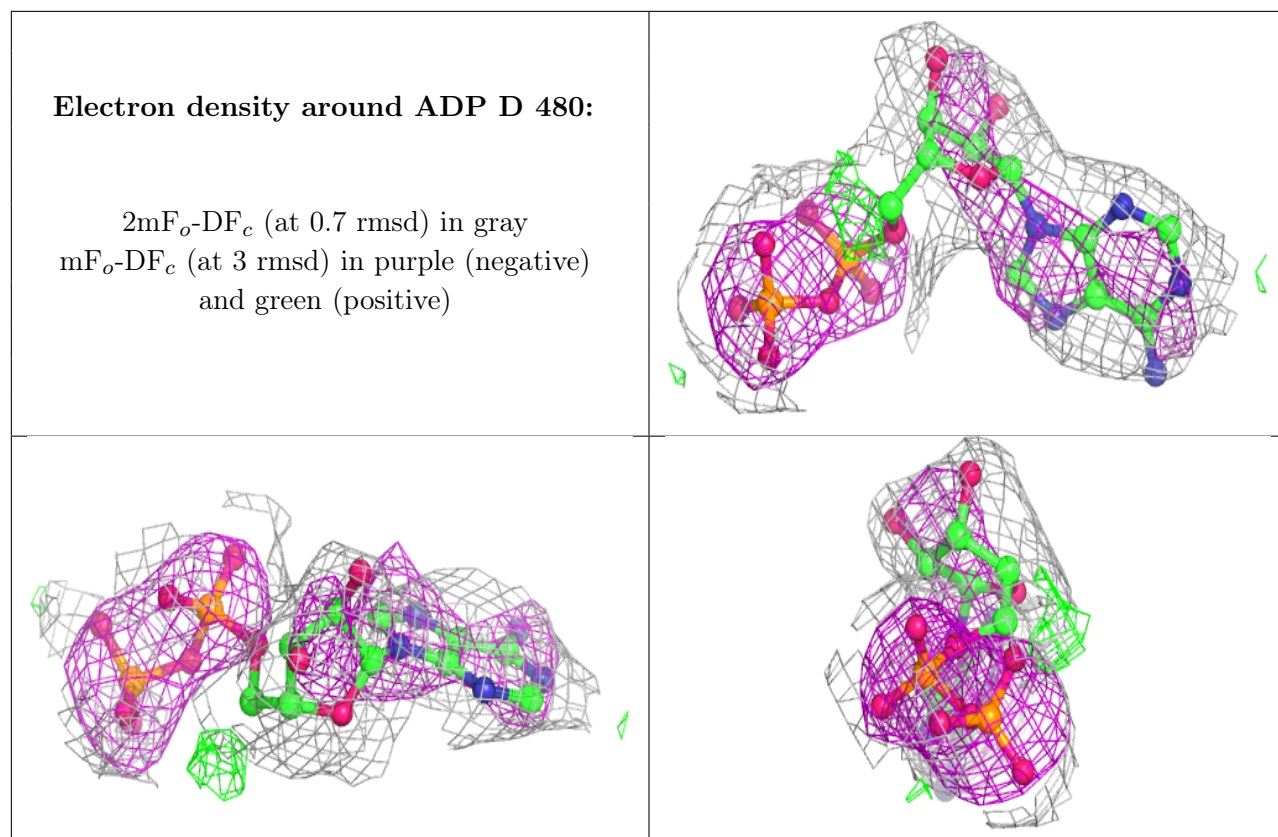## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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. 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	B-factors($Å^2$)	Q<0.9
3	ADP	B	480	27/27	0.92	0.17	85,89,89,90	0
3	ADP	D	480	27/27	0.92	0.17	84,91,92,92	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP B 480:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around ADP D 480:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.