



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:21 AM UTC

PDB ID : 5NBN / pdb_00005nbn
Title : Crystal structure of the Arp4-N-actin-Arp8-Ino80HSA module of INO80
Authors : Knoll, K.R.; Eustermann, S.; Hopfner, K.P.
Deposited on : 2017-03-02
Resolution : 4.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

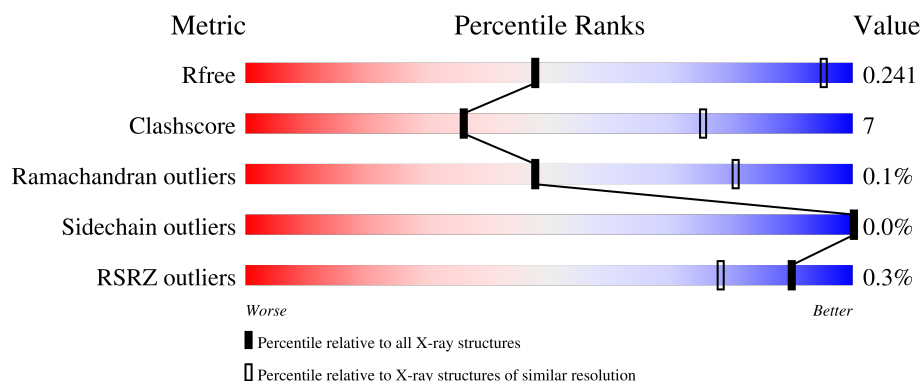
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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.



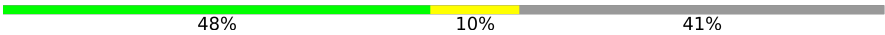
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 $\leq 5\%$. 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	489	 70% 13% 17%
1	B	489	 71% 12% 17%
2	C	375	 76% 19% .
2	D	375	 79% 17% .
3	E	628	 77% 18% 5%

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Mol	Chain	Length	Quality of chain
3	F	628	 76% 20% 5%
4	G	147	 51% 7% 41%
4	H	147	 48% 10% 41%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23215 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 Actin-related protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	16	0	0
			3160	2016	522	611	11			
1	B	406	Total	C	N	O	S	16	0	0
			3156	2014	522	609	11			

- Molecule 2 is a protein called Actin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	359	Total	C	N	O	S	0	0	0
			2798	1776	470	535	17			
2	D	359	Total	C	N	O	S	0	0	0
			2798	1776	470	535	17			

- Molecule 3 is a protein called Actin-like protein ARP8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	598	Total	C	N	O	S	0	0	0
			4818	3090	803	912	13			
3	F	598	Total	C	N	O	S	0	0	0
			4823	3094	804	912	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	254	MET	-	initiating methionine	UNP Q12386
F	254	MET	-	initiating methionine	UNP Q12386

- Molecule 4 is a protein called Putative DNA helicase INO80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	86	Total	C	N	O	S	0	0	0
			738	458	146	130	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	86	Total	C	N	O	S	0	0	0
			738	458	146	130	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	461	MET	-	initiating methionine	UNP P53115
G	599	ASN	-	expression tag	UNP P53115
G	600	TRP	-	expression tag	UNP P53115
G	601	SER	-	expression tag	UNP P53115
G	602	HIS	-	expression tag	UNP P53115
G	603	PRO	-	expression tag	UNP P53115
G	604	GLN	-	expression tag	UNP P53115
G	605	PHE	-	expression tag	UNP P53115
G	606	GLU	-	expression tag	UNP P53115
G	607	LYS	-	expression tag	UNP P53115
H	461	MET	-	initiating methionine	UNP P53115
H	599	ASN	-	expression tag	UNP P53115
H	600	TRP	-	expression tag	UNP P53115
H	601	SER	-	expression tag	UNP P53115
H	602	HIS	-	expression tag	UNP P53115
H	603	PRO	-	expression tag	UNP P53115
H	604	GLN	-	expression tag	UNP P53115
H	605	PHE	-	expression tag	UNP P53115
H	606	GLU	-	expression tag	UNP P53115
H	607	LYS	-	expression tag	UNP P53115

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

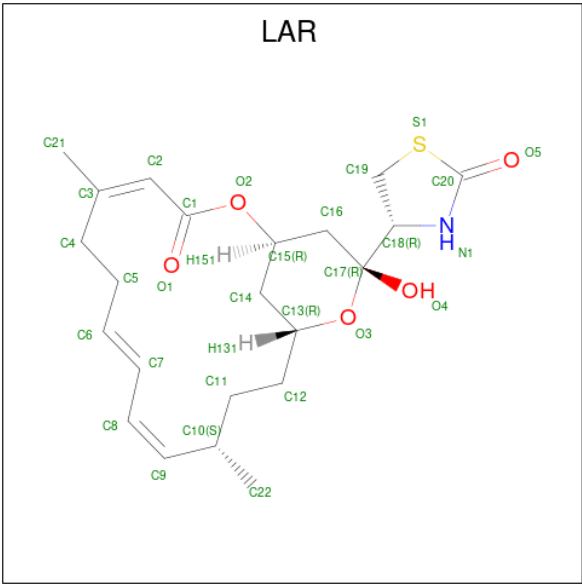
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 7 is LATRUNCULIN A (CCD ID: LAR) (formula: C₂₂H₃₁NO₅S).

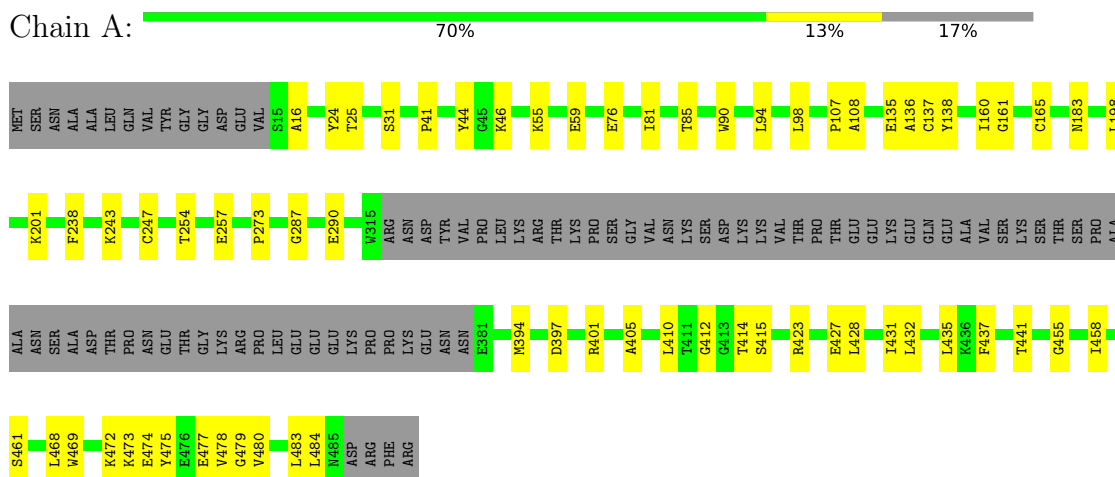


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	S	0	0
			29	22	1	5	1		
7	D	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

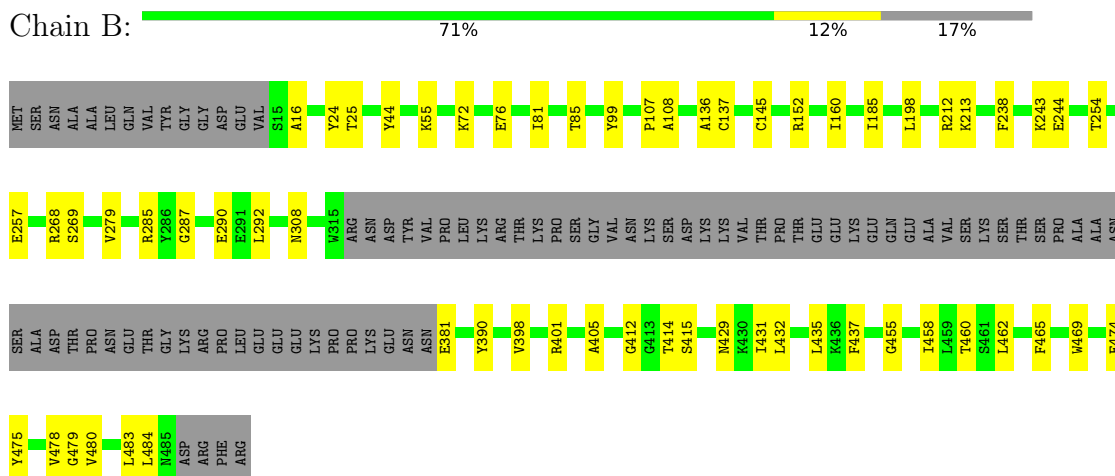
3 Residue-property plots

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.

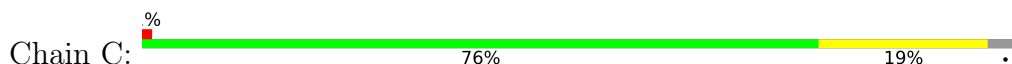
• Molecule 1: Actin-related protein 4

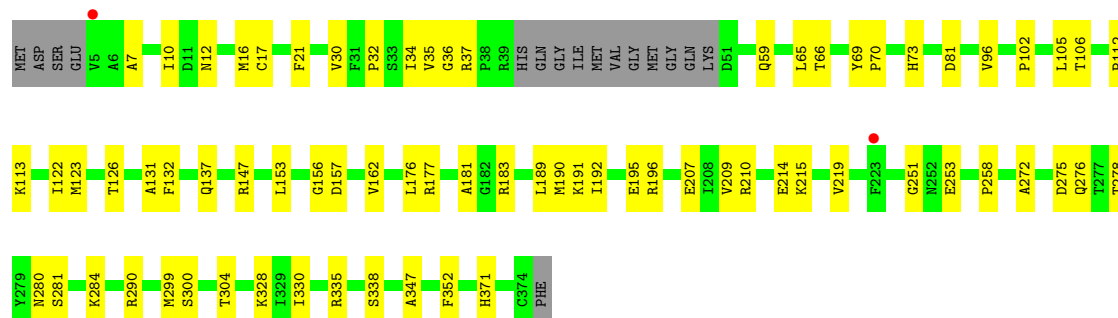


• Molecule 1: Actin-related protein 4



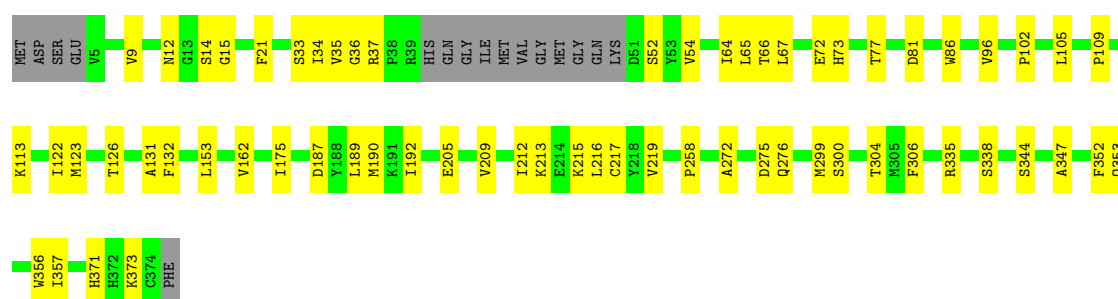
• Molecule 2: Actin





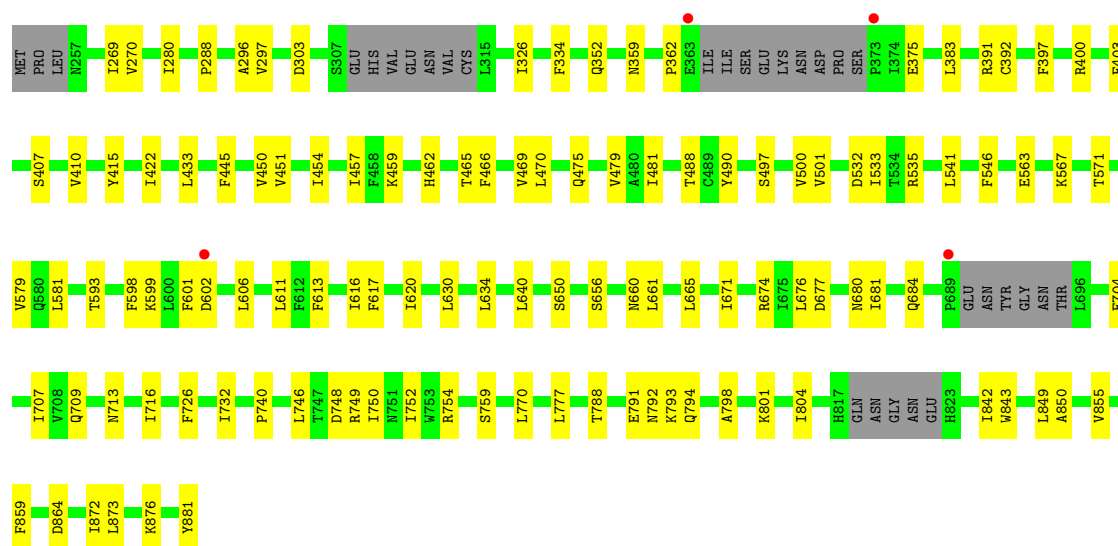
• Molecule 2: Actin

Chain D: 79% 17%



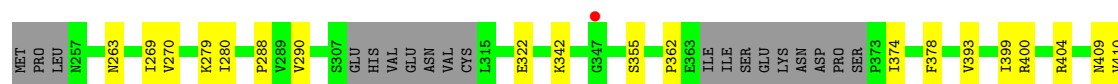
• Molecule 3: Actin-like protein ARP8

Chain E: 77% 18% 5%



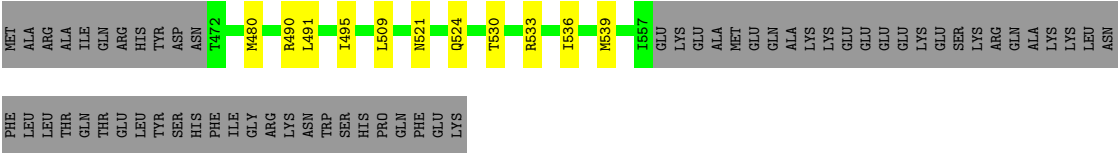
• Molecule 3: Actin-like protein ARP8

Chain F: 76% 20% 5%

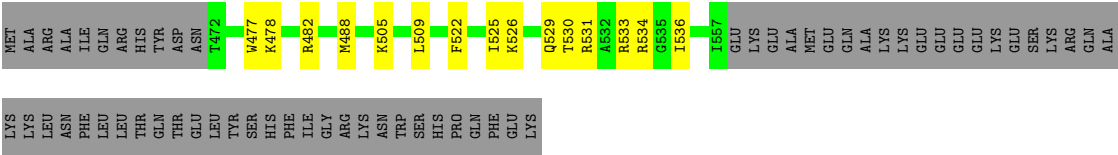




● Molecule 4: Putative DNA helicase INO80



● Molecule 4: Putative DNA helicase INO80



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	172.29Å 263.91Å 241.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 4.00 49.40 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.40-4.00) 99.9 (49.40-4.00)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.193 , 0.242 0.195 , 0.241	Depositor DCC
R_{free} test set	2380 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23215	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: CA, ATP, HIC, LAR

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	0.11	0/3229	0.29	0/4389
1	B	0.11	0/3225	0.30	0/4384
2	C	0.10	0/2846	0.30	0/3855
2	D	0.11	0/2846	0.31	0/3855
3	E	0.13	0/4924	0.33	0/6674
3	F	0.13	0/4929	0.33	0/6679
4	G	0.15	0/748	0.34	0/990
4	H	0.15	0/748	0.34	0/990
All	All	0.12	0/23495	0.32	0/31816

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	3160	0	3084	49	0
1	B	3156	0	3080	39	0
2	C	2798	0	2765	53	0
2	D	2798	0	2765	37	0
3	E	4818	0	4767	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	4823	0	4780	79	0
4	G	738	0	769	8	0
4	H	738	0	769	10	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	31	0	12	2	0
6	B	31	0	12	0	0
6	C	31	0	12	2	0
6	D	31	0	12	1	0
7	C	29	0	31	7	0
7	D	29	0	31	0	0
All	All	23215	0	22889	338	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 7.

All (338) 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)
2:C:16:MET:HA	2:C:32:PRO:HA	1.62	0.82
3:F:488:THR:HB	3:F:842:ILE:HD13	1.63	0.80
3:F:733:VAL:HG23	3:F:841:ILE:HD12	1.65	0.78
3:E:872:ILE:HD11	3:E:876:LYS:HD2	1.70	0.73
1:A:473:LYS:O	1:A:477:GLU:HB3	1.88	0.73
2:D:36:GLY:HA2	2:D:66:THR:O	1.90	0.72
3:E:488:THR:HB	3:E:842:ILE:HD13	1.71	0.72
2:D:122:ILE:O	2:D:126:THR:HB	1.91	0.71
2:C:59:GLN:HB2	7:C:503:LAR:H81	1.72	0.70
2:D:105:LEU:HD11	2:D:123:MET:HE3	1.74	0.70
4:G:530:THR:HG22	4:G:533:ARG:HH12	1.59	0.67
2:C:102:PRO:HB3	2:C:131:ALA:HB3	1.75	0.67
3:E:352:GLN:NE2	3:E:599:LYS:O	2.28	0.67
3:F:676:LEU:HD11	3:F:770:LEU:HD21	1.76	0.66
2:C:105:LEU:HD11	2:C:123:MET:HE3	1.77	0.66
3:F:280:ILE:HD11	3:F:433:LEU:HD13	1.79	0.65
1:B:480:VAL:HG22	1:B:483:LEU:H	1.61	0.65
2:C:122:ILE:O	2:C:126:THR:HB	1.98	0.64
3:E:533:ILE:HD11	3:E:611:LEU:HD21	1.79	0.63
3:E:788:THR:OG1	3:E:792:ASN:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:VAL:HG13	1:B:401:ARG:HH21	1.63	0.63
2:C:157:ASP:OD2	2:C:183:ARG:NH1	2.32	0.62
3:E:270:VAL:O	3:E:280:ILE:HA	2.00	0.61
3:E:501:VAL:HB	3:E:732:ILE:HD13	1.82	0.61
1:B:198:LEU:HD11	1:B:238:PHE:HE2	1.65	0.61
2:C:190:MET:HG2	2:C:209:VAL:HG21	1.83	0.60
7:C:503:LAR:O4	7:C:503:LAR:S1	2.59	0.60
3:E:459:LYS:HD2	3:E:462:HIS:CD2	2.37	0.60
1:B:465:PHE:HD2	4:G:480:MET:HE1	1.67	0.59
2:D:14:SER:N	6:D:502:ATP:O1G	2.36	0.59
3:F:832:PRO:HG3	3:F:841:ILE:HD11	1.84	0.58
2:C:34:ILE:HD12	7:C:503:LAR:H111	1.85	0.58
3:E:280:ILE:HD11	3:E:433:LEU:HD13	1.86	0.58
2:D:12:ASN:OD1	2:D:86:TRP:NE1	2.36	0.58
1:B:185:ILE:HG22	1:B:292:LEU:HD23	1.87	0.57
2:C:16:MET:HE2	2:C:30:VAL:HG12	1.86	0.57
2:D:102:PRO:HB3	2:D:131:ALA:HB3	1.87	0.57
3:E:535:ARG:HG2	3:E:620:ILE:HD12	1.86	0.57
1:A:480:VAL:HG22	1:A:483:LEU:H	1.70	0.57
2:C:272:ALA:HB1	2:C:276:GLN:HB2	1.86	0.57
2:C:32:PRO:HB3	7:C:503:LAR:H141	1.87	0.57
3:F:270:VAL:O	3:F:280:ILE:HA	2.05	0.56
4:H:478:LYS:HG3	4:H:482:ARG:HE	1.70	0.56
3:E:297:VAL:HG22	3:E:383:LEU:HD22	1.86	0.56
2:C:113:LYS:HB3	2:C:371:HIS:CE1	2.40	0.56
2:D:219:VAL:HG22	2:D:258:PRO:HB2	1.87	0.56
3:E:676:LEU:HD11	3:E:770:LEU:HD21	1.86	0.56
3:F:488:THR:HG21	3:F:500:VAL:HG11	1.87	0.56
3:E:433:LEU:HD23	3:E:445:PHE:CE1	2.42	0.55
2:C:105:LEU:HD12	2:C:132:PHE:HE1	1.72	0.55
2:D:35:VAL:HG21	2:D:81:ASP:HB3	1.89	0.55
3:E:400:ARG:HD2	3:E:415:TYR:CZ	2.41	0.55
1:A:431:ILE:HG13	1:A:432:LEU:HG	1.88	0.55
3:F:400:ARG:HD2	3:F:415:TYR:CZ	2.42	0.55
3:E:793:LYS:HE2	3:E:793:LYS:HA	1.88	0.55
1:B:475:TYR:O	1:B:479:GLY:HA2	2.07	0.54
2:C:157:ASP:HB2	6:C:502:ATP:H5'1	1.88	0.54
2:C:219:VAL:HG22	2:C:258:PRO:HB2	1.88	0.54
3:E:288:PRO:HB3	3:E:843:TRP:CE2	2.41	0.54
1:A:31:SER:HB2	1:A:461:SER:HB2	1.89	0.54
3:E:704:GLU:OE1	3:E:749:ARG:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:288:PRO:HB3	3:F:843:TRP:CE2	2.41	0.54
3:F:263:ASN:HA	3:F:449:LYS:HE2	1.89	0.54
3:F:704:GLU:OE1	3:F:749:ARG:HB3	2.08	0.54
2:C:21:PHE:HE1	2:C:96:VAL:HG11	1.72	0.54
1:A:475:TYR:O	1:A:479:GLY:HA2	2.08	0.54
1:B:287:GLY:HA2	1:B:290:GLU:HB3	1.90	0.53
2:D:36:GLY:O	2:D:52:SER:OG	2.26	0.53
2:D:153:LEU:HD13	2:D:162:VAL:HG22	1.91	0.53
2:D:212:ILE:HG23	2:D:216:LEU:HD12	1.90	0.53
2:C:299:MET:HE2	2:C:304:THR:HB	1.90	0.53
3:E:571:THR:HA	3:E:740:PRO:HD2	1.90	0.53
1:A:394:MET:O	1:A:401:ARG:NH1	2.42	0.53
3:F:400:ARG:HH12	3:F:420:GLU:HG2	1.74	0.53
3:F:411:LYS:HA	3:F:626:LYS:HA	1.90	0.52
1:B:107:PRO:HB3	1:B:136:ALA:HB3	1.90	0.52
2:D:272:ALA:HB1	2:D:276:GLN:HB2	1.90	0.52
3:F:832:PRO:HG3	3:F:841:ILE:CD1	2.39	0.52
1:A:431:ILE:O	1:A:432:LEU:HD23	2.09	0.52
1:B:16:ALA:HB3	1:B:460:THR:HG21	1.91	0.52
4:H:530:THR:HG22	4:H:533:ARG:HH12	1.75	0.52
1:B:405:ALA:O	1:B:437:PHE:HA	2.09	0.52
2:D:109:PRO:HB3	2:D:175:ILE:HD13	1.92	0.52
3:E:410:VAL:HG13	3:E:630:LEU:HD12	1.92	0.52
3:F:677:ASP:O	3:F:681:ILE:HG13	2.10	0.52
3:F:754:ARG:HH11	3:F:759:SER:HA	1.75	0.52
2:D:105:LEU:HD12	2:D:132:PHE:HE1	1.75	0.52
3:E:656:SER:HA	3:E:661:LEU:HD21	1.92	0.52
2:D:299:MET:HE2	2:D:304:THR:HB	1.92	0.51
3:F:269:ILE:HD13	3:F:433:LEU:HD11	1.92	0.51
3:F:355:SER:HB3	3:F:547:PRO:HB3	1.91	0.51
2:C:328:LYS:HE3	2:C:330:ILE:HD11	1.92	0.51
4:H:533:ARG:O	4:H:536:ILE:HG22	2.11	0.51
1:B:55:LYS:NZ	1:B:85:THR:OG1	2.43	0.51
2:D:353:GLN:O	2:D:356:TRP:NE1	2.43	0.51
3:F:784:ALA:O	3:F:788:THR:HG23	2.10	0.51
3:E:296:ALA:HB1	3:E:397:PHE:CD1	2.46	0.51
2:C:196:ARG:HH22	2:C:251:GLY:HA3	1.76	0.50
3:F:660:ASN:HB3	3:F:674:ARG:HH11	1.77	0.50
3:F:288:PRO:HD2	3:F:840:LEU:HD13	1.92	0.50
3:E:392:CYS:HB3	3:E:397:PHE:CD1	2.46	0.50
3:E:855:VAL:HB	3:E:859:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:490:TYR:HE1	4:G:536:ILE:HG22	1.77	0.50
2:D:15:GLY:O	2:D:33:SER:CB	2.60	0.50
1:A:455:GLY:HA2	1:A:458:ILE:HG22	1.94	0.49
3:F:409:ASN:ND2	3:F:412:SER:HB2	2.27	0.49
3:F:533:ILE:HD11	3:F:611:LEU:HD21	1.94	0.49
3:F:656:SER:HA	3:F:661:LEU:HD21	1.93	0.49
1:A:397:ASP:O	1:A:401:ARG:HG3	2.12	0.49
1:A:432:LEU:HD12	1:A:437:PHE:HZ	1.77	0.49
1:A:473:LYS:O	1:A:477:GLU:CB	2.60	0.49
2:C:113:LYS:HB3	2:C:371:HIS:HE1	1.77	0.49
3:F:788:THR:HG22	3:F:793:LYS:HD3	1.94	0.49
3:F:868:HIS:HB2	3:F:872:ILE:HG23	1.94	0.49
3:F:613:PHE:O	3:F:616:ILE:HG22	2.12	0.49
3:F:836:MET:HE2	3:F:844:LYS:HE2	1.95	0.49
1:B:268:ARG:HD3	1:B:285:ARG:NH1	2.28	0.49
1:A:24:TYR:HD2	1:A:25:THR:HG23	1.78	0.49
1:B:145:CYS:O	1:B:455:GLY:HA3	2.13	0.49
2:C:280:ASN:O	2:C:284:LYS:HG2	2.11	0.49
3:E:326:ILE:HG21	3:E:616:ILE:HB	1.95	0.49
4:G:533:ARG:O	4:G:536:ILE:HG13	2.12	0.49
2:C:10:ILE:HB	2:C:105:LEU:HD23	1.95	0.49
3:E:457:ILE:HD11	3:E:650:SER:HB2	1.95	0.49
3:E:754:ARG:HH11	3:E:759:SER:HA	1.76	0.49
3:F:660:ASN:HB3	3:F:674:ARG:NH1	2.28	0.49
3:F:761:ALA:HB3	3:F:823:HIS:HD2	1.77	0.49
1:A:287:GLY:HA2	1:A:290:GLU:HB3	1.95	0.48
2:D:335:ARG:HA	2:D:338:SER:OG	2.13	0.48
3:F:850:ALA:HA	3:F:855:VAL:HG11	1.96	0.48
1:B:308:ASN:O	1:B:381:GLU:N	2.47	0.48
2:C:300:SER:HA	2:C:335:ARG:HB2	1.96	0.48
2:D:15:GLY:O	2:D:33:SER:HB2	2.12	0.48
2:D:72:GLU:HG3	2:D:77:THR:HG21	1.94	0.48
3:E:677:ASP:O	3:E:681:ILE:HG13	2.13	0.48
2:D:357:ILE:HG12	2:D:373:LYS:HG3	1.95	0.48
2:C:12:ASN:HA	2:C:17:CYS:HB2	1.95	0.48
3:E:454:ILE:HD12	3:E:481:ILE:HB	1.94	0.48
3:F:670:LYS:HE2	3:F:674:ARG:NH2	2.29	0.48
4:G:521:ASN:OD1	4:G:524:GLN:HB2	2.14	0.48
2:C:214:GLU:HG2	6:C:502:ATP:C5	2.49	0.47
1:A:138:TYR:CD2	1:A:468:LEU:HD21	2.49	0.47
3:E:602:ASP:O	3:E:606:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:433:LEU:HD23	3:F:445:PHE:CE1	2.49	0.47
2:C:335:ARG:HA	2:C:338:SER:OG	2.13	0.47
3:E:407:SER:HB3	3:E:462:HIS:HD2	1.78	0.47
3:F:451:VAL:HG21	3:F:850:ALA:HB2	1.96	0.47
2:C:36:GLY:HA2	2:C:66:THR:O	2.13	0.47
2:C:215:LYS:NZ	3:E:475:GLN:OE1	2.40	0.47
3:E:488:THR:HG21	3:E:500:VAL:HG11	1.95	0.47
3:F:399:ILE:CG2	3:F:556:LYS:HD3	2.45	0.47
3:F:342:LYS:HG2	3:F:574:ASP:HB3	1.96	0.47
3:F:374:ILE:HD12	3:F:587:ARG:HG2	1.95	0.47
1:A:432:LEU:HB2	1:A:437:PHE:HE2	1.80	0.47
3:E:375:GLU:O	3:E:391:ARG:NH1	2.48	0.47
1:B:24:TYR:HD2	1:B:25:THR:HG23	1.79	0.47
3:E:269:ILE:HD13	3:E:433:LEU:HD11	1.96	0.47
3:F:487:ALA:O	3:F:845:GLY:HA3	2.14	0.47
2:D:275:ASP:OD1	2:D:275:ASP:N	2.49	0.46
2:D:300:SER:HA	2:D:335:ARG:HB2	1.97	0.46
3:E:798:ALA:HA	3:E:801:LYS:HE2	1.97	0.46
3:E:850:ALA:HA	3:E:855:VAL:HG11	1.98	0.46
3:E:359:ASN:HA	3:E:593:THR:O	2.15	0.46
3:F:734:GLY:O	3:F:737:SER:OG	2.25	0.46
1:B:431:ILE:HG13	1:B:432:LEU:HG	1.97	0.46
3:F:754:ARG:NH1	3:F:825:PHE:HB2	2.29	0.46
3:F:869:GLY:O	3:F:872:ILE:HG12	2.15	0.46
3:E:777:LEU:HD11	3:E:804:ILE:HG13	1.98	0.46
3:F:579:VAL:HA	3:F:601:PHE:HB2	1.97	0.46
3:F:855:VAL:HB	3:F:859:PHE:CE2	2.51	0.46
4:H:526:LYS:HA	4:H:529:GLN:HG2	1.98	0.46
1:A:198:LEU:HD11	1:A:238:PHE:HE2	1.81	0.46
2:D:187:ASP:HA	2:D:190:MET:HE2	1.98	0.46
1:B:16:ALA:HB2	1:B:107:PRO:HG2	1.98	0.46
2:C:70:PRO:HB3	2:C:81:ASP:HB2	1.97	0.46
3:E:296:ALA:HB1	3:E:397:PHE:HD1	1.80	0.46
3:E:661:LEU:HD22	3:E:709:GLN:HG3	1.98	0.46
3:F:279:LYS:HG3	3:F:290:VAL:HG22	1.97	0.46
3:E:791:GLU:O	3:E:794:GLN:NE2	2.49	0.46
1:B:244:GLU:OE1	2:C:290:ARG:NH2	2.49	0.46
2:C:147:ARG:CZ	2:C:330:ILE:HD13	2.46	0.46
4:H:505:LYS:HE3	4:H:509:LEU:HD11	1.98	0.45
2:D:347:ALA:HA	2:D:352:PHE:CD2	2.51	0.45
3:F:587:ARG:HG3	3:F:588:SER:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:275:ASP:OD1	2:C:275:ASP:N	2.49	0.45
3:E:746:LEU:HD23	3:E:746:LEU:HA	1.84	0.45
1:B:160:ILE:HG22	1:B:414:THR:HB	1.99	0.45
3:F:454:ILE:HD12	3:F:481:ILE:HB	1.99	0.45
2:C:7:ALA:HB3	2:C:347:ALA:HB1	1.99	0.45
3:F:450:VAL:HB	3:F:479:VAL:HG22	1.98	0.45
3:F:668:ASP:HB3	3:F:757:LEU:HD22	1.99	0.45
1:A:243:LYS:HA	1:A:247:CYS:SG	2.57	0.45
3:E:707:ILE:HD12	3:E:750:ILE:HD11	1.99	0.44
1:A:243:LYS:NZ	6:A:502:ATP:O2'	2.29	0.44
2:C:189:LEU:HA	2:C:192:ILE:HG12	1.99	0.44
3:E:532:ASP:HB3	3:E:617:PHE:CD1	2.52	0.44
3:F:811:GLN:O	3:F:815:ILE:HG12	2.17	0.44
1:A:16:ALA:HB2	1:A:107:PRO:HG2	1.99	0.44
1:B:432:LEU:HD13	1:B:435:LEU:HD12	1.99	0.44
1:A:55:LYS:NZ	1:A:85:THR:OG1	2.46	0.44
3:E:665:LEU:HD12	3:E:671:ILE:HG12	1.99	0.44
3:F:482:ILE:HD12	3:F:849:LEU:HG	2.00	0.44
1:A:24:TYR:CD2	1:A:25:THR:HG23	2.52	0.44
4:G:491:LEU:O	4:G:495:ILE:HG12	2.16	0.44
4:H:531:ARG:O	4:H:534:ARG:HG2	2.18	0.44
2:C:59:GLN:CB	7:C:503:LAR:H81	2.45	0.44
2:D:213:LYS:HA	2:D:217:CYS:SG	2.58	0.44
3:F:378:PHE:CE2	3:F:393:VAL:HG11	2.53	0.44
1:B:76:GLU:HB2	1:B:81:ILE:HD13	2.00	0.44
1:B:108:ALA:O	1:B:137:CYS:HA	2.17	0.44
1:B:474:GLU:O	1:B:478:VAL:HG22	2.17	0.44
3:F:754:ARG:HH12	3:F:825:PHE:HB2	1.83	0.44
3:F:777:LEU:HD11	3:F:804:ILE:HG13	1.99	0.44
3:E:497:SER:HB2	3:E:726:PHE:CE1	2.53	0.44
3:E:660:ASN:HB3	3:E:674:ARG:HH11	1.82	0.44
1:B:412:GLY:O	1:B:415:SER:OG	2.22	0.44
2:C:156:GLY:O	2:C:181:ALA:HB1	2.18	0.44
2:D:21:PHE:HE1	2:D:96:VAL:HG11	1.83	0.44
1:A:135:GLU:O	1:A:472:LYS:HG3	2.18	0.43
1:A:238:PHE:CD1	1:A:273:PRO:HD3	2.53	0.43
1:A:474:GLU:O	1:A:478:VAL:HG22	2.18	0.43
7:C:503:LAR:H131	7:C:503:LAR:H71	2.00	0.43
3:E:864:ASP:HB3	3:E:872:ILE:HD12	2.00	0.43
2:C:37:ARG:O	2:C:65:LEU:HA	2.18	0.43
3:F:404:ARG:HG3	3:F:409:ASN:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ALA:O	1:A:137:CYS:HA	2.17	0.43
2:C:191:LYS:O	2:C:195:GLU:HG3	2.18	0.43
3:E:450:VAL:HB	3:E:479:VAL:HG22	2.01	0.43
3:F:773:GLU:CD	3:F:808:LEU:HD11	2.43	0.43
1:A:160:ILE:HG22	1:A:414:THR:HB	2.00	0.43
3:E:579:VAL:HA	3:E:601:PHE:HB2	1.99	0.43
1:A:136:ALA:HB1	1:A:469:TRP:HB3	2.00	0.43
1:A:254:THR:HG23	1:A:257:GLU:H	1.84	0.43
3:E:465:THR:O	3:E:469:VAL:HG23	2.19	0.43
3:F:712:ALA:O	3:F:715:SER:OG	2.33	0.43
1:A:405:ALA:O	1:A:437:PHE:HA	2.19	0.43
3:E:462:HIS:CE1	3:E:634:LEU:HD13	2.53	0.43
1:A:41:PRO:HD3	1:A:59:GLU:HB2	2.01	0.43
3:F:465:THR:O	3:F:469:VAL:HG23	2.19	0.43
1:A:427:GLU:O	1:A:431:ILE:HG12	2.19	0.43
2:C:196:ARG:HG2	2:D:64:ILE:HG23	2.00	0.43
2:D:189:LEU:HA	2:D:192:ILE:HG12	2.00	0.43
3:E:288:PRO:HB3	3:E:843:TRP:CD2	2.53	0.43
3:E:303:ASP:OD1	3:E:303:ASP:N	2.52	0.43
3:F:532:ASP:HB3	3:F:617:PHE:CD1	2.54	0.43
1:A:76:GLU:HB2	1:A:81:ILE:HD13	2.01	0.42
1:A:138:TYR:CG	1:A:468:LEU:HD21	2.53	0.42
3:F:429:LEU:O	3:F:433:LEU:HB2	2.19	0.42
3:E:541:LEU:O	3:E:546:PHE:HB2	2.19	0.42
3:E:334:PHE:CE2	3:E:602:ASP:HB2	2.54	0.42
3:E:680:ASN:O	3:E:684:GLN:HB2	2.20	0.42
2:C:162:VAL:HG11	2:C:278:THR:HA	2.01	0.42
3:E:451:VAL:HG21	3:E:850:ALA:HB2	2.00	0.42
3:E:490:TYR:HE2	3:E:849:LEU:HD23	1.84	0.42
3:F:452:LEU:HD22	3:F:453:VAL:H	1.84	0.42
1:A:201:LYS:HE3	1:A:201:LYS:HB2	1.84	0.42
1:A:480:VAL:HG13	1:A:484:LEU:HD13	2.02	0.42
2:C:35:VAL:HG21	2:C:81:ASP:HB3	2.01	0.42
3:F:793:LYS:O	3:F:796:LEU:HB3	2.19	0.42
1:A:44:TYR:CD2	1:A:55:LYS:HD3	2.54	0.42
1:B:24:TYR:CD2	1:B:25:THR:HG23	2.53	0.42
1:B:243:LYS:HE2	1:B:243:LYS:HB3	1.81	0.42
3:E:433:LEU:HD12	3:E:433:LEU:HA	1.85	0.42
3:F:584:PHE:CE1	3:F:596:TYR:HB2	2.54	0.42
3:F:754:ARG:NH1	3:F:759:SER:HA	2.35	0.42
3:F:761:ALA:HB3	3:F:823:HIS:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:TYR:CD1	1:B:85:THR:HG21	2.55	0.42
3:F:540:PHE:HB3	3:F:603:GLU:OE2	2.20	0.42
3:F:844:LYS:O	3:F:847:SER:OG	2.28	0.42
4:H:529:GLN:HG3	4:H:530:THR:N	2.34	0.42
1:A:290:GLU:OE1	1:A:423:ARG:NH1	2.47	0.42
3:E:748:ASP:O	3:E:752:ILE:HG13	2.20	0.42
3:F:733:VAL:HG22	3:F:838:PRO:O	2.20	0.42
3:E:422:ILE:HD13	3:E:422:ILE:HA	1.93	0.41
3:F:490:TYR:HE2	3:F:849:LEU:HD23	1.85	0.41
2:D:213:LYS:HD2	2:D:306:PHE:HZ	1.85	0.41
3:E:581:LEU:HD22	3:E:598:PHE:O	2.20	0.41
3:F:679:HIS:HA	3:F:682:ILE:HG12	2.02	0.41
1:A:161:GLY:HA3	6:A:502:ATP:O1G	2.19	0.41
1:A:405:ALA:HB2	1:A:435:LEU:HD13	2.01	0.41
1:A:428:LEU:O	1:A:432:LEU:N	2.45	0.41
2:C:207:GLU:OE1	2:C:210:ARG:NH2	2.53	0.41
1:A:410:LEU:HB3	1:A:441:THR:HG22	2.02	0.41
2:D:113:LYS:HB3	2:D:371:HIS:NE2	2.35	0.41
1:B:99:TYR:OH	2:C:177:ARG:NH1	2.53	0.41
2:D:35:VAL:HA	2:D:54:VAL:HG12	2.01	0.41
1:A:31:SER:CB	1:A:461:SER:HB2	2.51	0.41
1:B:152:ARG:NH2	4:G:490:ARG:HH21	2.19	0.41
1:B:212:ARG:NH1	1:B:213:LYS:HE3	2.36	0.41
2:C:196:ARG:HG2	2:C:196:ARG:O	2.20	0.41
2:C:330:ILE:HG23	3:E:640:LEU:HD22	2.02	0.41
1:B:44:TYR:CE1	1:B:72:LYS:HB2	2.56	0.41
1:B:136:ALA:HB1	1:B:469:TRP:HB3	2.03	0.41
1:B:269:SER:HB3	1:B:279:VAL:HG22	2.03	0.41
1:B:390:TYR:HB2	1:B:431:ILE:HD12	2.02	0.41
2:C:190:MET:HG3	2:C:209:VAL:HG11	2.03	0.41
2:C:196:ARG:HD2	2:C:253:GLU:OE2	2.21	0.41
3:E:613:PHE:O	3:E:616:ILE:HG22	2.20	0.41
3:F:801:LYS:HB3	3:F:801:LYS:HE2	1.85	0.41
4:H:522:PHE:HA	4:H:525:ILE:HG22	2.02	0.41
1:B:99:TYR:CD2	2:C:112:PRO:HG3	2.56	0.41
1:B:458:ILE:O	1:B:462:LEU:HB2	2.21	0.41
1:B:480:VAL:HG13	1:B:484:LEU:HD13	2.03	0.41
3:F:322:GLU:HB3	3:F:619:LEU:HD21	2.02	0.41
1:A:44:TYR:CG	1:A:85:THR:HG21	2.56	0.41
1:A:90:TRP:O	1:A:94:LEU:HG	2.21	0.41
1:A:165:CYS:HB3	1:A:183:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:HD13	4:H:477:TRP:HE1	1.86	0.41
2:C:69:TYR:OH	7:C:503:LAR:H112	2.20	0.41
2:C:347:ALA:HA	2:C:352:PHE:CD2	2.56	0.41
2:D:34:ILE:HD11	2:D:67:LEU:HD22	2.03	0.41
3:E:403:PHE:HZ	3:E:466:PHE:HE1	1.67	0.41
3:E:466:PHE:HE2	3:E:470:LEU:HD11	1.85	0.41
3:F:557:HIS:NE2	3:F:587:ARG:O	2.54	0.41
4:G:539:MET:HE3	4:G:539:MET:HB3	1.93	0.41
1:B:254:THR:HG23	1:B:257:GLU:H	1.86	0.41
2:C:106:THR:HB	2:C:137:GLN:HG2	2.03	0.41
3:E:297:VAL:HG21	3:E:400:ARG:HE	1.86	0.41
3:E:563:GLU:O	3:E:567:LYS:HB2	2.21	0.41
3:F:342:LYS:N	3:F:342:LYS:HD2	2.35	0.41
3:F:651:LEU:HB2	3:F:682:ILE:HG22	2.03	0.41
2:C:153:LEU:HD13	2:C:162:VAL:HG22	2.03	0.40
2:D:37:ARG:O	2:D:65:LEU:HA	2.22	0.40
3:E:873:LEU:HD13	3:E:881:TYR:CE1	2.56	0.40
1:A:94:LEU:HD23	1:A:98:LEU:HD22	2.03	0.40
2:D:215:LYS:HG3	3:F:472:THR:O	2.21	0.40
4:H:488:MET:HE2	4:H:488:MET:HB2	1.92	0.40
2:D:9:VAL:HG21	2:D:344:SER:HA	2.03	0.40
3:E:713:ASN:HA	3:E:716:ILE:HG12	2.02	0.40
3:F:873:LEU:HD13	3:F:881:TYR:CE1	2.55	0.40
1:A:46:LYS:HD3	1:A:55:LYS:HG2	2.03	0.40
1:B:429:ASN:HD22	1:B:429:ASN:HA	1.74	0.40
2:C:176:LEU:HD12	2:C:281:SER:HB2	2.03	0.40
2:D:205:GLU:O	2:D:209:VAL:HG23	2.21	0.40
3:F:748:ASP:O	3:F:752:ILE:HG13	2.21	0.40
1:A:412:GLY:O	1:A:415:SER:OG	2.30	0.40
3:F:410:VAL:HA	3:F:630:LEU:HD22	2.03	0.40
3:F:592:PRO:O	3:F:594:GLU:HG3	2.21	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	402/489 (82%)	387 (96%)	15 (4%)	0	100	100
1	B	402/489 (82%)	387 (96%)	15 (4%)	0	100	100
2	C	354/375 (94%)	349 (99%)	5 (1%)	0	100	100
2	D	354/375 (94%)	348 (98%)	6 (2%)	0	100	100
3	E	588/628 (94%)	558 (95%)	29 (5%)	1 (0%)	43	75
3	F	588/628 (94%)	557 (95%)	30 (5%)	1 (0%)	43	75
4	G	84/147 (57%)	82 (98%)	2 (2%)	0	100	100
4	H	84/147 (57%)	83 (99%)	1 (1%)	0	100	100
All	All	2856/3278 (87%)	2751 (96%)	103 (4%)	2 (0%)	48	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	362	PRO
3	F	362	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	345/434 (80%)	345 (100%)	0	100	100
1	B	344/434 (79%)	344 (100%)	0	100	100
2	C	305/319 (96%)	305 (100%)	0	100	100
2	D	305/319 (96%)	305 (100%)	0	100	100
3	E	540/574 (94%)	540 (100%)	0	100	100
3	F	541/574 (94%)	541 (100%)	0	100	100
4	G	81/136 (60%)	80 (99%)	1 (1%)	63	73
4	H	81/136 (60%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2542/2926 (87%)	2541 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	509	LEU

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	406	HIS
1	B	60	GLN
1	B	154	ASN
1	B	248	HIS
1	B	429	ASN
2	C	87	HIS
2	C	232	GLN
2	D	246	GLN
3	E	462	HIS
3	E	549	GLN
3	E	724	ASN
3	E	851	GLN
3	F	316	GLN
3	F	319	GLN
3	F	409	ASN
3	F	729	ASN
4	G	496	GLN
4	H	502	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
2	HIC	D	73	2	10,11,12	1.57	2 (20%)	9,14,16	1.27	1 (11%)
2	HIC	C	73	2	10,11,12	1.55	1 (10%)	9,14,16	1.27	1 (11%)

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	HIC	D	73	2	-	2/5/6/8	0/1/1/1
2	HIC	C	73	2	-	4/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	73	HIC	CD2-CG	3.18	1.41	1.36
2	C	73	HIC	CD2-CG	3.09	1.41	1.36
2	D	73	HIC	CD2-NE2	2.06	1.40	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	73	HIC	NE2-CE1-ND1	-3.32	111.39	112.66
2	C	73	HIC	NE2-CE1-ND1	-3.03	111.50	112.66

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	73	HIC	C-CA-CB-CG
2	C	73	HIC	CA-CB-CG-CD2
2	D	73	HIC	CA-CB-CG-CD2
2	C	73	HIC	CA-CB-CG-ND1
2	D	73	HIC	CA-CB-CG-ND1
2	C	73	HIC	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
6	ATP	C	502	5	32,33,33	1.42	5 (15%)	48,52,52	1.76	9 (18%)
6	ATP	A	502	5	32,33,33	1.39	4 (12%)	48,52,52	1.77	8 (16%)
7	LAR	C	503	-	30,31,31	4.93	15 (50%)	32,43,43	5.15	11 (34%)
7	LAR	D	503	-	30,31,31	4.92	15 (50%)	32,43,43	5.50	12 (37%)
6	ATP	D	502	5	32,33,33	1.41	5 (15%)	48,52,52	1.72	9 (18%)
6	ATP	B	502	5	32,33,33	1.40	4 (12%)	48,52,52	1.73	10 (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
6	ATP	C	502	5	-	7/22/38/38	0/3/3/3
6	ATP	A	502	5	-	4/22/38/38	0/3/3/3
7	LAR	C	503	-	-	3/23/51/51	0/2/3/3
7	LAR	D	503	-	-	10/23/51/51	0/2/3/3
6	ATP	D	502	5	-	7/22/38/38	0/3/3/3
6	ATP	B	502	5	-	7/22/38/38	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	503	LAR	C2-C3	14.75	1.60	1.33
7	C	503	LAR	C2-C3	14.71	1.59	1.33
7	C	503	LAR	C20-S1	-10.13	1.56	1.77
7	D	503	LAR	C20-S1	-10.06	1.56	1.77
7	C	503	LAR	C18-N1	8.57	1.57	1.46
7	D	503	LAR	C18-N1	8.39	1.57	1.46
7	C	503	LAR	C7-C6	7.40	1.58	1.33
7	D	503	LAR	C7-C6	7.36	1.58	1.33
7	C	503	LAR	C19-S1	-7.13	1.64	1.81
7	D	503	LAR	C19-S1	-7.00	1.64	1.81
7	C	503	LAR	C8-C9	6.73	1.58	1.33
7	D	503	LAR	C17-C18	-6.71	1.41	1.54
7	D	503	LAR	C8-C9	6.70	1.58	1.33
7	C	503	LAR	C17-C18	-6.52	1.42	1.54
7	C	503	LAR	O2-C1	5.76	1.46	1.34
7	D	503	LAR	O2-C1	5.63	1.46	1.34
6	A	502	ATP	C5-C4	4.80	1.47	1.39
7	D	503	LAR	O3-C17	4.75	1.51	1.43
6	D	502	ATP	C5-C4	4.71	1.47	1.39
6	C	502	ATP	C5-C4	4.70	1.47	1.39
7	C	503	LAR	C2-C1	4.68	1.57	1.46
6	B	502	ATP	C5-C4	4.64	1.47	1.39
7	D	503	LAR	C2-C1	4.58	1.57	1.46
7	C	503	LAR	O3-C17	4.52	1.50	1.43
7	D	503	LAR	C19-C18	4.10	1.62	1.52
7	C	503	LAR	C19-C18	4.05	1.62	1.52
7	D	503	LAR	C8-C7	3.36	1.54	1.44
7	C	503	LAR	C8-C7	3.36	1.54	1.44
7	C	503	LAR	C4-C3	3.22	1.57	1.51
7	D	503	LAR	C4-C3	3.21	1.57	1.51
6	D	502	ATP	C5-C6	2.78	1.48	1.41
6	C	502	ATP	C5-C6	2.76	1.48	1.41
6	B	502	ATP	C5-C6	2.73	1.48	1.41
6	A	502	ATP	C5-C6	2.69	1.48	1.41
7	D	503	LAR	O5-C20	-2.62	1.18	1.22
7	C	503	LAR	O5-C20	-2.56	1.18	1.22
7	D	503	LAR	C12-C11	2.48	1.59	1.53
7	C	503	LAR	C12-C11	2.46	1.59	1.53
6	B	502	ATP	C8-N7	2.42	1.36	1.31
6	C	502	ATP	C8-N7	2.42	1.36	1.31
6	D	502	ATP	C8-N7	2.36	1.36	1.31
6	A	502	ATP	C5-N7	-2.35	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	502	ATP	C5-N7	-2.23	1.35	1.39
6	A	502	ATP	C8-N7	2.23	1.36	1.31
6	D	502	ATP	C5-N7	-2.23	1.35	1.39
6	B	502	ATP	C5-N7	-2.17	1.35	1.39
6	D	502	ATP	PB-O3B	2.05	1.61	1.59
6	C	502	ATP	PB-O3B	2.01	1.61	1.59

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	503	LAR	C19-S1-C20	23.23	105.49	92.04
7	C	503	LAR	C19-S1-C20	20.53	103.93	92.04
7	D	503	LAR	O4-C17-O3	-12.64	85.46	110.00
7	C	503	LAR	O4-C17-O3	-12.51	85.71	110.00
7	D	503	LAR	O3-C17-C18	11.10	118.49	104.25
7	C	503	LAR	O3-C17-C18	10.90	118.23	104.25
7	C	503	LAR	O4-C17-C16	-8.04	83.90	109.80
7	D	503	LAR	O4-C17-C16	-7.61	85.26	109.80
6	A	502	ATP	C5-C4-N3	-5.92	118.56	126.72
6	D	502	ATP	C5-C4-N3	-5.86	118.65	126.72
6	C	502	ATP	C5-C4-N3	-5.84	118.67	126.72
6	B	502	ATP	C5-C4-N3	-5.66	118.93	126.72
6	A	502	ATP	N3-C4-N9	4.80	135.33	127.17
7	C	503	LAR	O2-C1-C2	4.76	122.24	111.20
6	D	502	ATP	N3-C4-N9	4.55	134.90	127.17
7	D	503	LAR	O2-C1-C2	4.53	121.70	111.20
6	C	502	ATP	N3-C4-N9	4.52	134.86	127.17
6	B	502	ATP	N3-C4-N9	4.38	134.61	127.17
6	D	502	ATP	C2-N3-C4	3.70	120.87	111.83
6	C	502	ATP	C2-N3-C4	3.70	120.86	111.83
6	B	502	ATP	C2-N3-C4	3.68	120.83	111.83
6	A	502	ATP	C2-N3-C4	3.65	120.75	111.83
6	C	502	ATP	C4-C5-N7	-3.58	106.48	110.58
6	B	502	ATP	C4-C5-N7	-3.55	106.52	110.58
6	D	502	ATP	C4-C5-N7	-3.54	106.54	110.58
7	C	503	LAR	O1-C1-C2	-3.41	117.74	126.23
6	A	502	ATP	C4-C5-N7	-3.32	106.79	110.58
6	B	502	ATP	N3-C2-N1	-3.27	123.63	128.58
6	C	502	ATP	N3-C2-N1	-3.22	123.72	128.58
7	D	503	LAR	O1-C1-C2	-3.19	118.28	126.23
6	D	502	ATP	N3-C2-N1	-3.19	123.76	128.58
6	A	502	ATP	N3-C2-N1	-3.09	123.91	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	503	LAR	C11-C12-C13	-2.99	108.61	114.06
7	C	503	LAR	C14-C13-C12	-2.84	108.01	113.28
6	B	502	ATP	C4-N9-C8	2.70	108.57	105.74
7	D	503	LAR	O3-C13-C14	2.65	113.69	109.02
6	C	502	ATP	C5-N7-C8	2.58	107.51	103.45
6	C	502	ATP	C4-N9-C8	2.56	108.42	105.74
6	A	502	ATP	C4-N9-C8	2.56	108.42	105.74
6	B	502	ATP	C5-N7-C8	2.55	107.46	103.45
7	D	503	LAR	C12-C11-C10	-2.53	109.86	114.11
6	D	502	ATP	C4-N9-C8	2.52	108.38	105.74
6	D	502	ATP	C5-N7-C8	2.47	107.34	103.45
7	C	503	LAR	O3-C13-C14	2.47	113.36	109.02
6	A	502	ATP	C3'-C2'-C1'	2.41	106.02	101.46
6	A	502	ATP	C5-N7-C8	2.40	107.22	103.45
6	B	502	ATP	C3'-C2'-C1'	2.39	105.97	101.46
7	D	503	LAR	C14-C13-C12	-2.30	109.02	113.28
6	B	502	ATP	C6-C5-N7	2.24	136.41	132.09
7	C	503	LAR	C12-C11-C10	-2.16	110.48	114.11
6	C	502	ATP	C6-C5-N7	2.15	136.24	132.09
7	C	503	LAR	C21-C3-C4	2.15	118.95	115.23
7	D	503	LAR	O2-C1-O1	-2.08	120.02	123.34
6	B	502	ATP	N9-C8-N7	-2.07	110.99	113.94
7	C	503	LAR	O2-C1-O1	-2.07	120.02	123.34
6	D	502	ATP	C6-C5-N7	2.07	136.09	132.09
6	C	502	ATP	C3'-C2'-C1'	2.06	105.36	101.46
6	D	502	ATP	C3'-C2'-C1'	2.04	105.33	101.46
7	D	503	LAR	C21-C3-C4	2.02	118.73	115.23

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	ATP	C5'-O5'-PA-O2A
6	A	502	ATP	C5'-O5'-PA-O3A
6	B	502	ATP	C5'-O5'-PA-O3A
6	C	502	ATP	C5'-O5'-PA-O1A
6	C	502	ATP	C5'-O5'-PA-O3A
6	D	502	ATP	C5'-O5'-PA-O1A
6	D	502	ATP	C5'-O5'-PA-O3A
7	D	503	LAR	O3-C17-C18-C19
7	D	503	LAR	C3-C4-C5-C6
7	C	503	LAR	C11-C12-C13-O3

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Mol	Chain	Res	Type	Atoms
7	D	503	LAR	C11-C12-C13-O3
6	B	502	ATP	O4'-C4'-C5'-O5'
6	B	502	ATP	C3'-C4'-C5'-O5'
7	D	503	LAR	C21-C3-C4-C5
6	A	502	ATP	O4'-C4'-C5'-O5'
7	D	503	LAR	C4-C5-C6-C7
7	C	503	LAR	C4-C5-C6-C7
6	A	502	ATP	C3'-C4'-C5'-O5'
7	D	503	LAR	C2-C3-C4-C5
7	D	503	LAR	C10-C11-C12-C13
6	B	502	ATP	C5'-O5'-PA-O1A
6	C	502	ATP	C5'-O5'-PA-O2A
6	D	502	ATP	C5'-O5'-PA-O2A
6	B	502	ATP	PB-O3A-PA-O1A
6	C	502	ATP	PG-O3B-PB-O2B
6	C	502	ATP	PB-O3A-PA-O1A
7	D	503	LAR	C6-C7-C8-C9
7	D	503	LAR	O2-C1-C2-C3
7	C	503	LAR	O2-C1-C2-C3
6	C	502	ATP	PG-O3B-PB-O1B
6	C	502	ATP	PB-O3A-PA-O2A
6	D	502	ATP	PG-O3B-PB-O1B
6	D	502	ATP	PB-O3A-PA-O1A
7	D	503	LAR	C11-C12-C13-C14
6	B	502	ATP	PA-O3A-PB-O1B
6	B	502	ATP	PA-O3A-PB-O2B
6	D	502	ATP	PG-O3B-PB-O2B
6	D	502	ATP	PB-O3A-PA-O2A

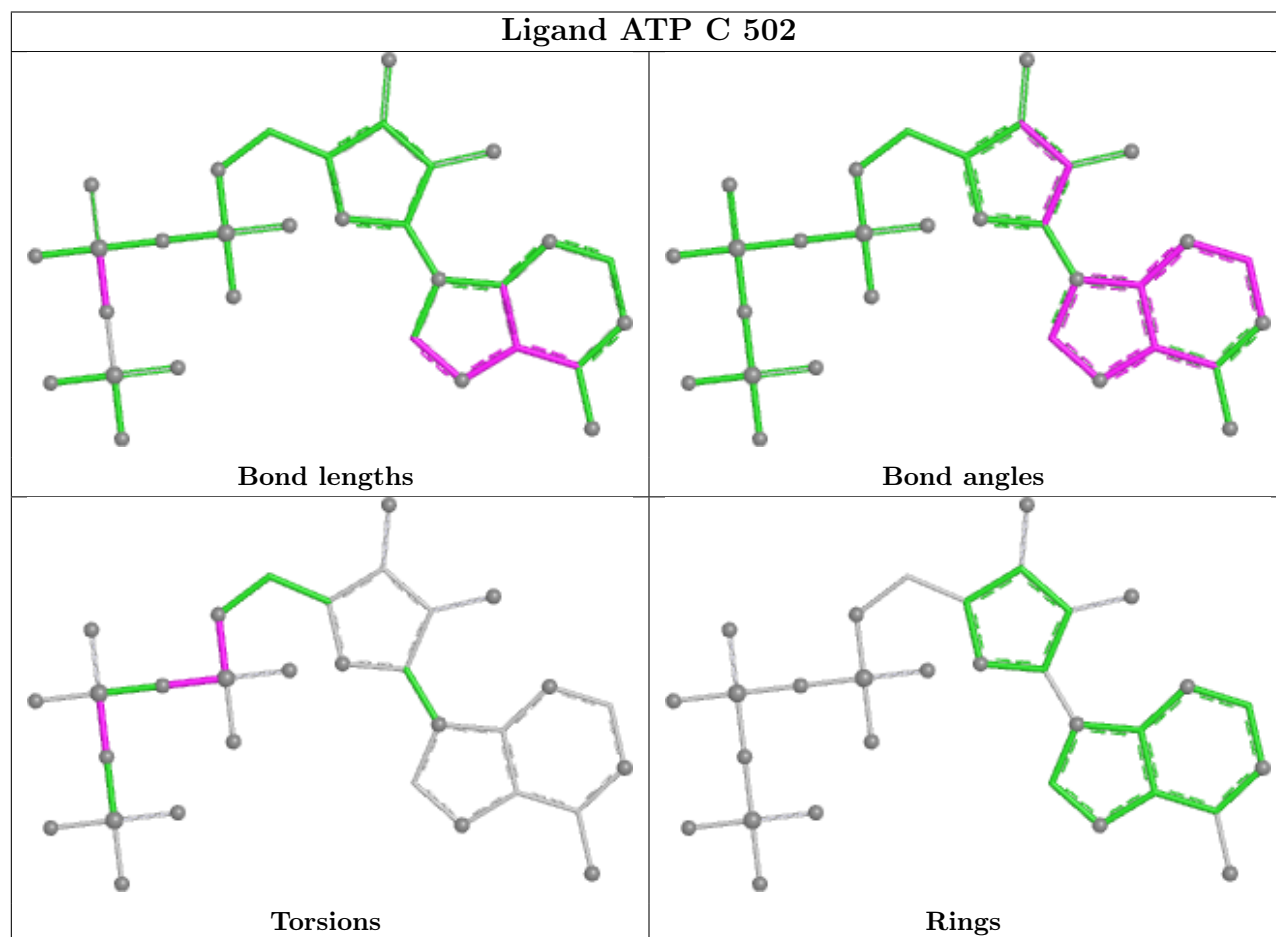
There are no ring outliers.

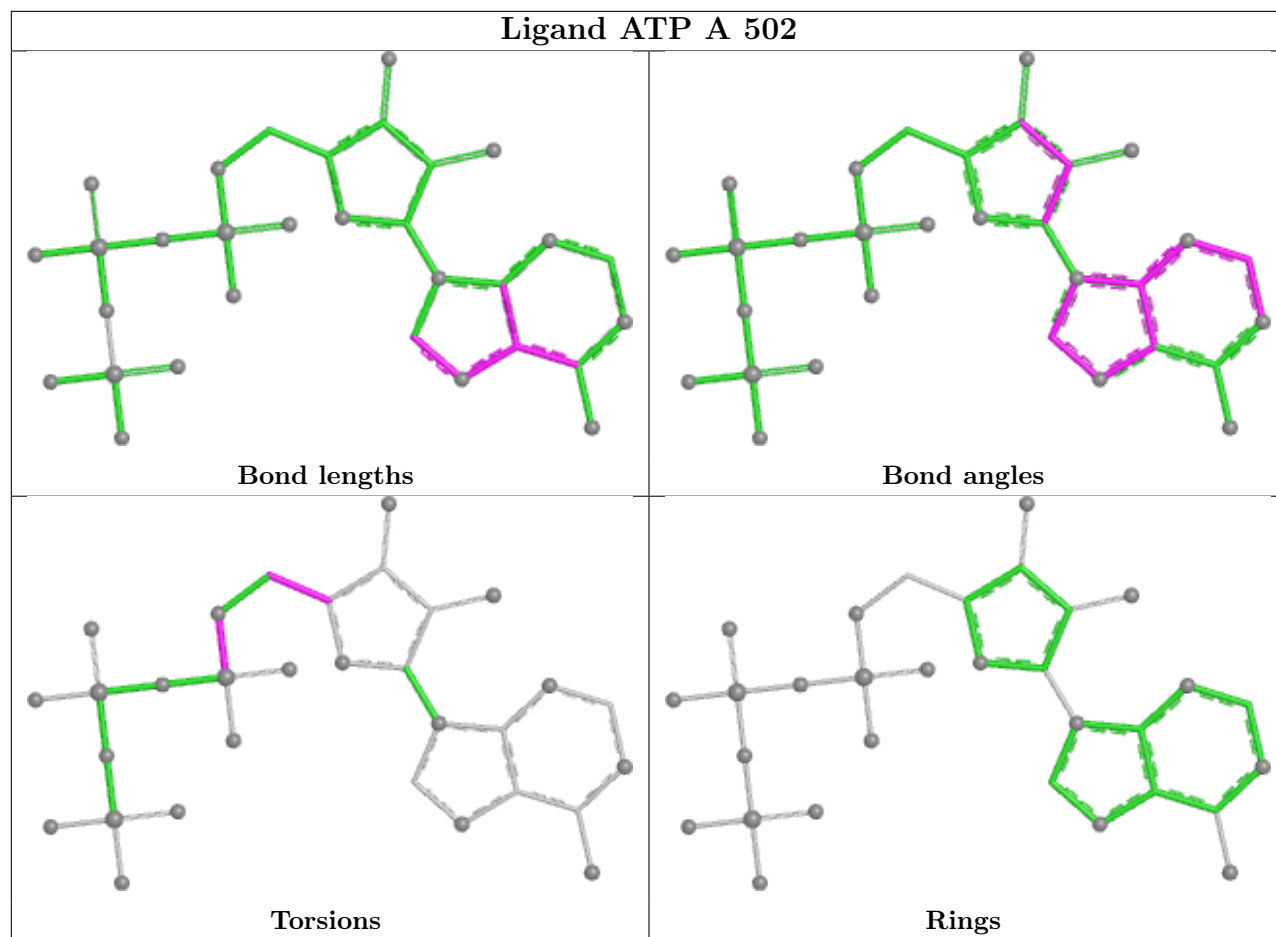
4 monomers are involved in 12 short contacts:

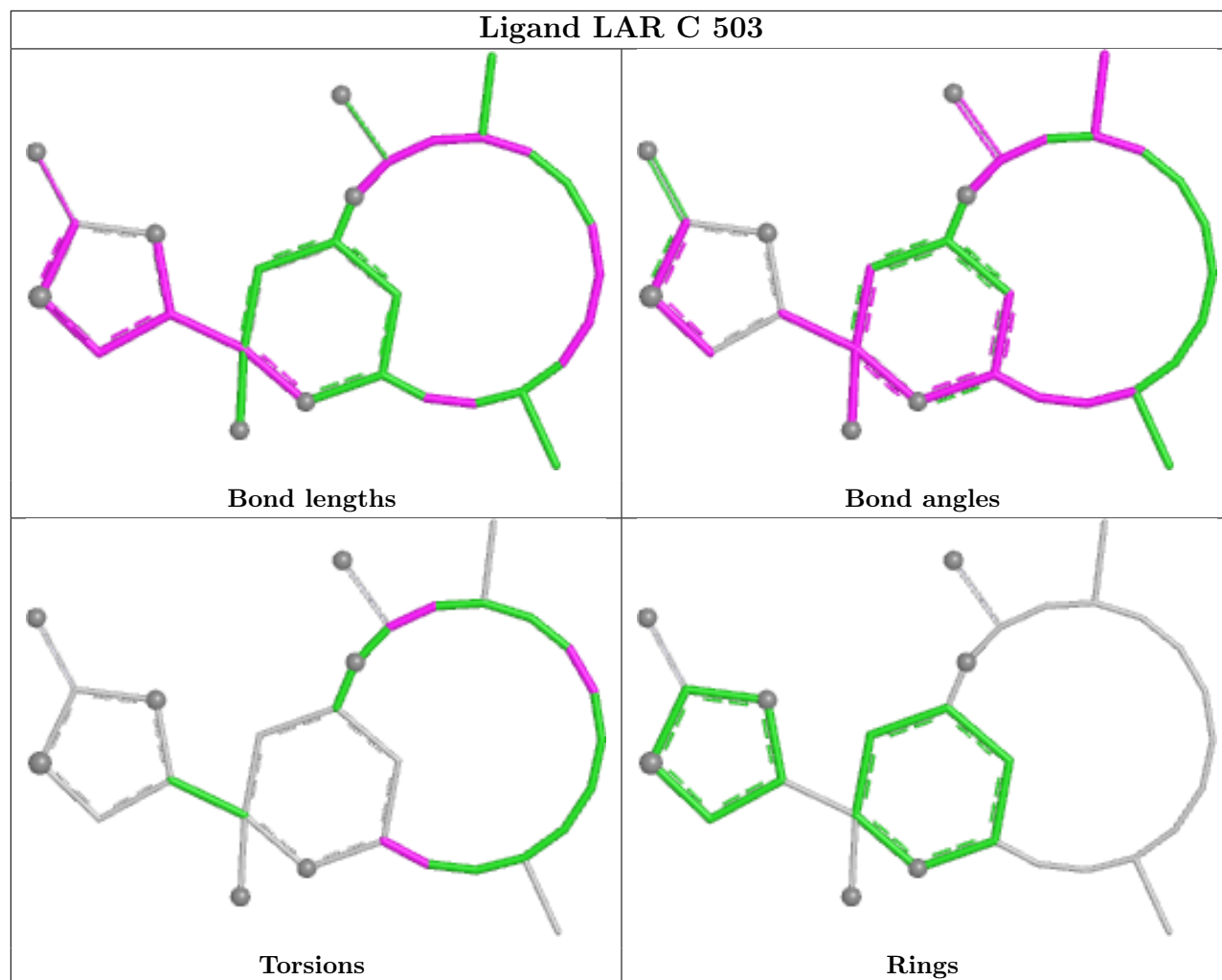
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	502	ATP	2	0
6	A	502	ATP	2	0
7	C	503	LAR	7	0
6	D	502	ATP	1	0

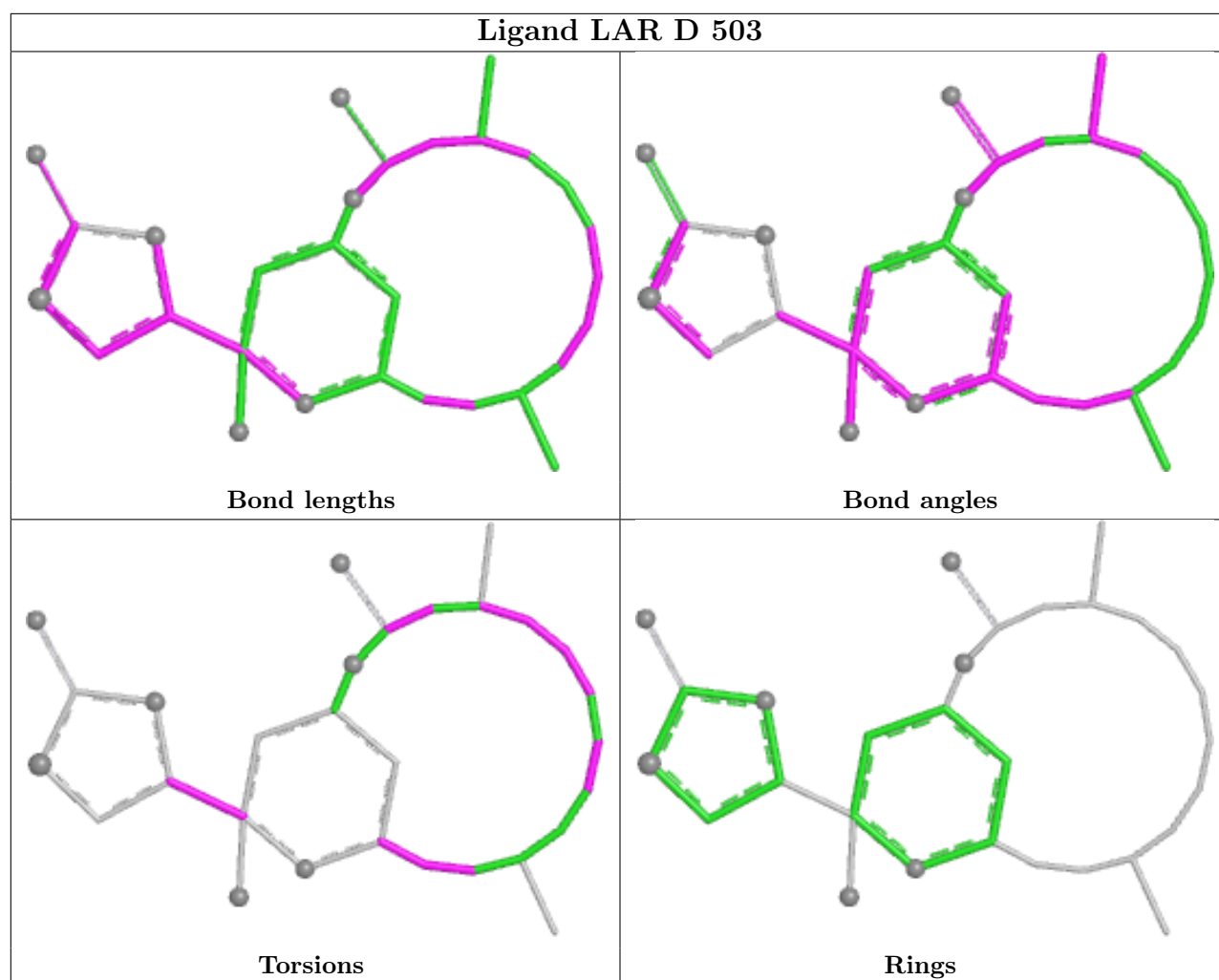
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

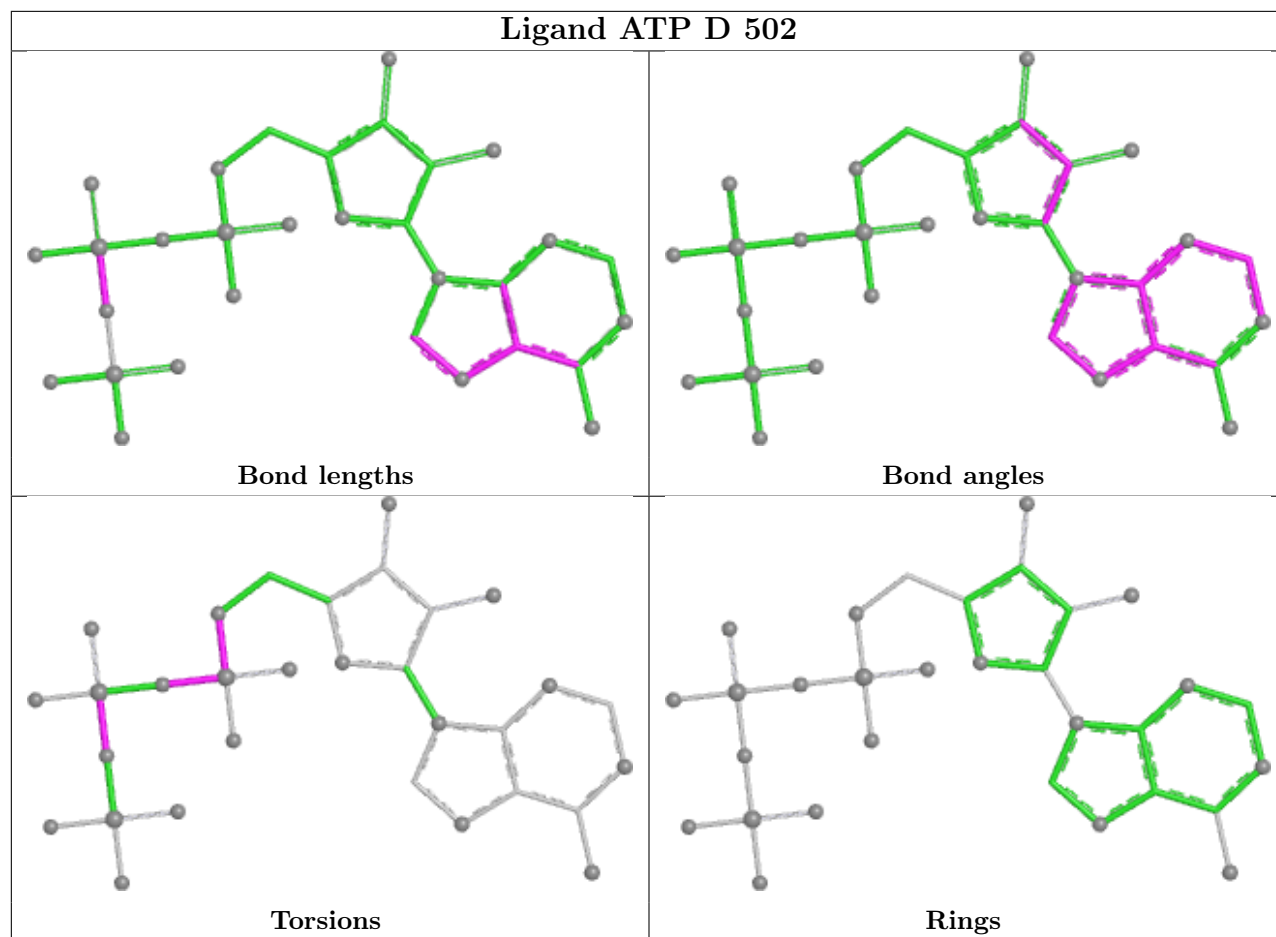
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

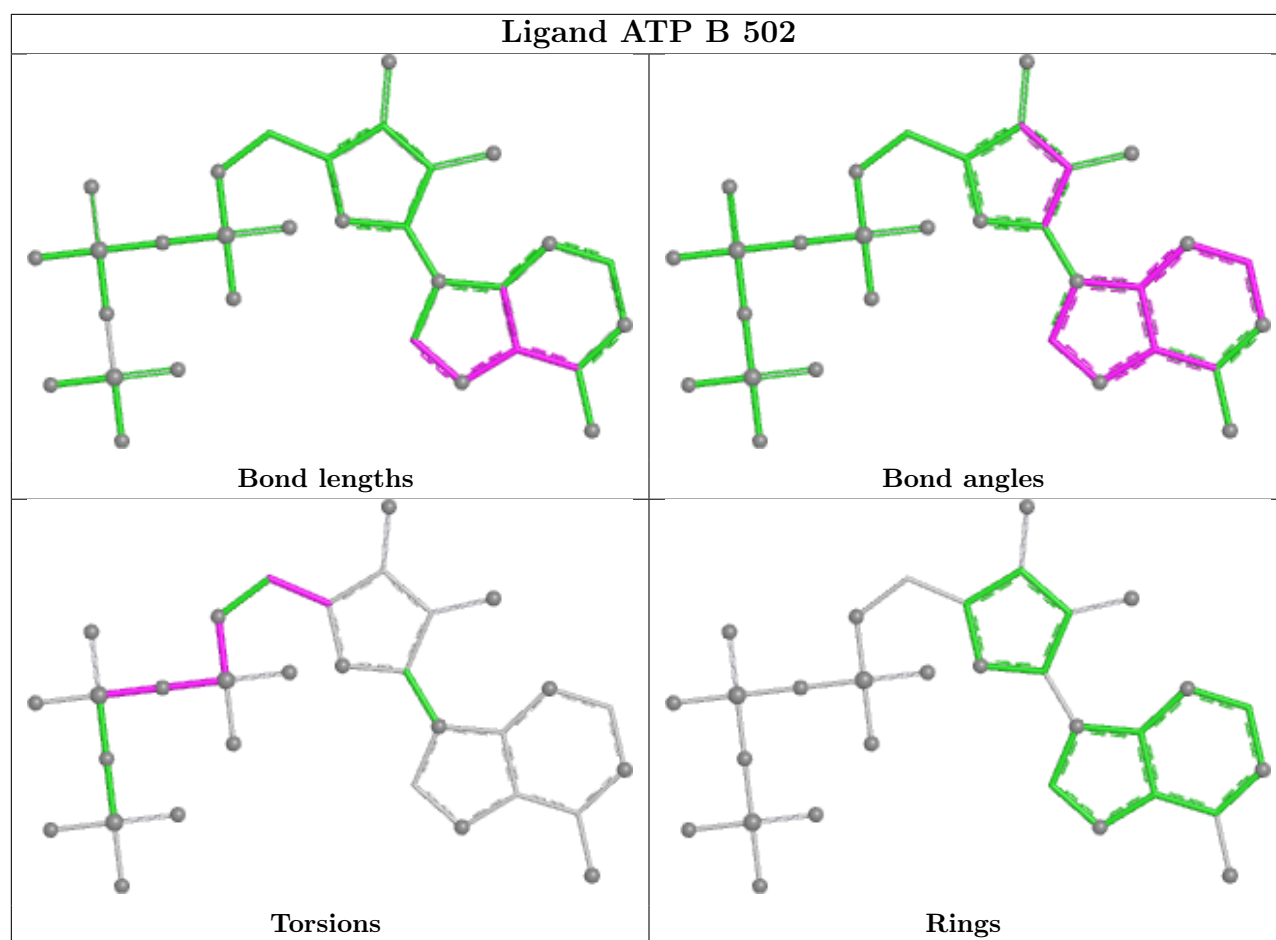












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	406/489 (83%)	-0.17	0 100 100	69, 121, 174, 224	4 (0%)
1	B	406/489 (83%)	-0.17	0 100 100	71, 136, 182, 219	4 (0%)
2	C	358/375 (95%)	-0.26	2 (0%) 85 71	66, 101, 145, 187	0
2	D	358/375 (95%)	-0.35	0 100 100	53, 88, 128, 163	0
3	E	598/628 (95%)	-0.07	4 (0%) 84 68	63, 125, 189, 232	0
3	F	598/628 (95%)	-0.13	2 (0%) 90 78	54, 120, 189, 231	0
4	G	86/147 (58%)	-0.20	0 100 100	81, 126, 165, 199	0
4	H	86/147 (58%)	-0.24	0 100 100	68, 117, 162, 179	0
All	All	2896/3278 (88%)	-0.18	8 (0%) 90 78	53, 118, 179, 232	8 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	363	GLU	3.0
3	E	373	PRO	2.7
3	F	347	GLY	2.5
2	C	5	VAL	2.3
3	E	689	PRO	2.3
3	E	602	ASP	2.2
2	C	223	PHE	2.1
3	F	668	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
2	HIC	D	73	11/12	0.90	0.12	84,96,122,142	0
2	HIC	C	73	11/12	0.91	0.12	89,119,130,131	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

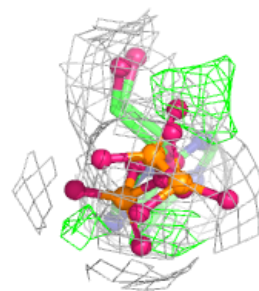
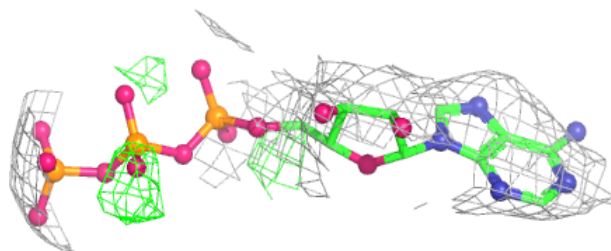
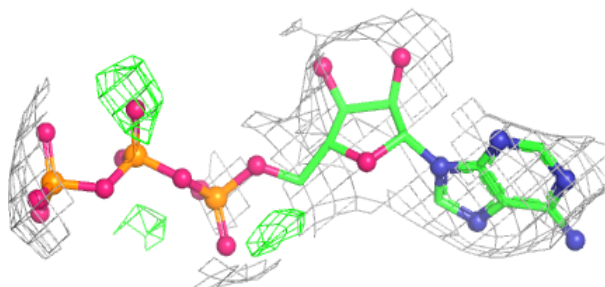
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	B	501	1/1	0.93	0.17	143,143,143,143	0
6	ATP	B	502	31/31	0.94	0.10	90,107,165,177	0
7	LAR	D	503	29/29	0.94	0.11	70,99,116,126	0
5	CA	D	501	1/1	0.96	0.13	62,62,62,62	0
6	ATP	C	502	31/31	0.96	0.10	60,96,116,129	0
7	LAR	C	503	29/29	0.96	0.10	105,114,133,145	0
6	ATP	A	502	31/31	0.96	0.09	70,96,130,153	0
6	ATP	D	502	31/31	0.97	0.07	56,73,89,99	0
5	CA	A	501	1/1	0.97	0.09	117,117,117,117	0
5	CA	C	501	1/1	0.97	0.07	74,74,74,74	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.

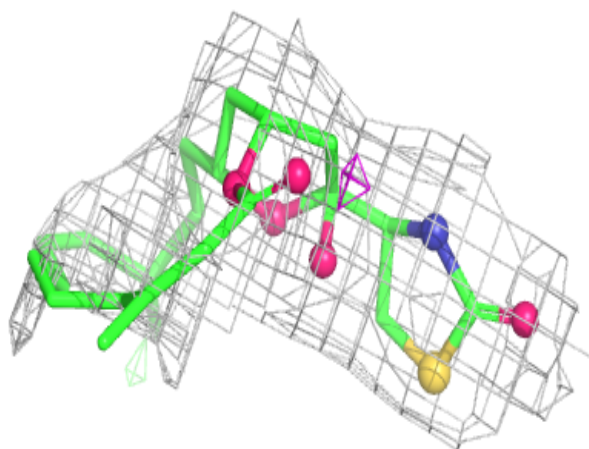
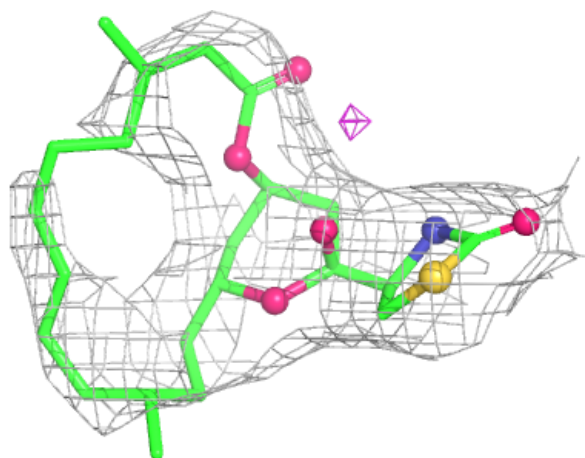
Electron density around ATP B 502:

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



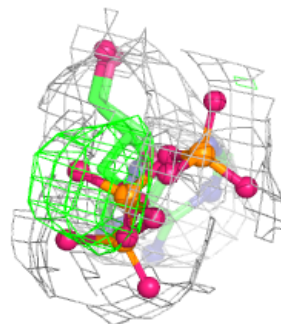
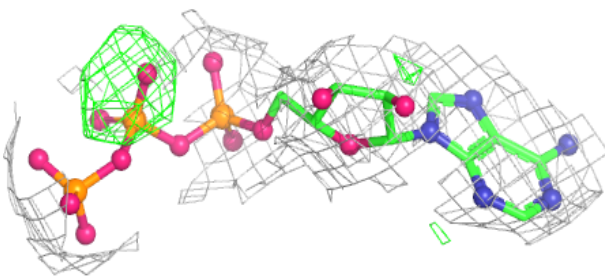
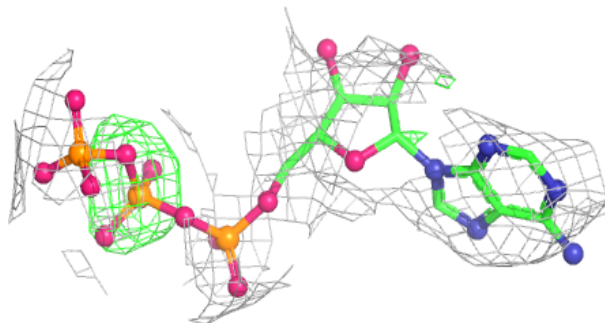
Electron density around LAR D 503:

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



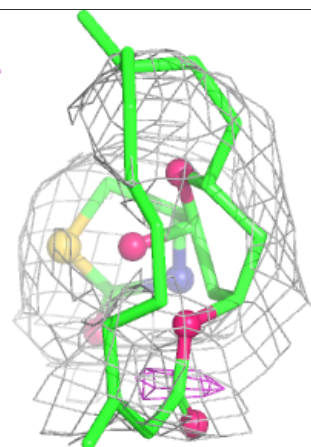
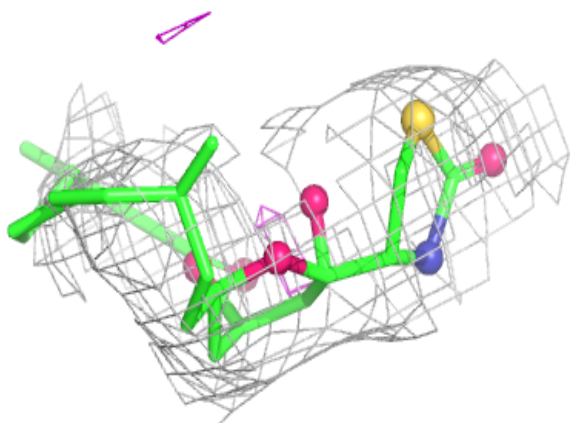
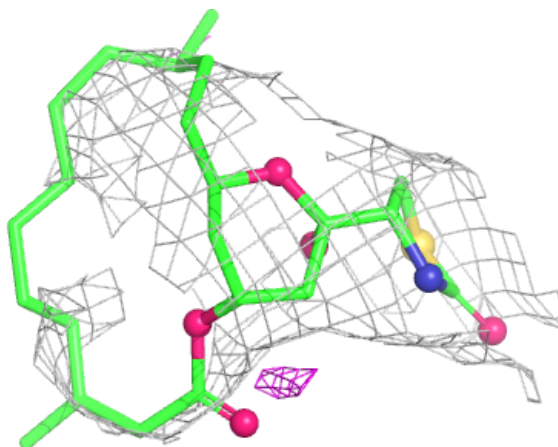
Electron density around ATP C 502:

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



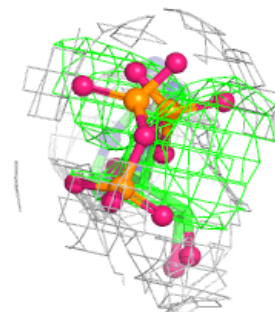
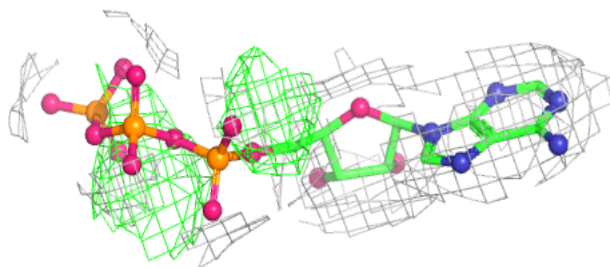
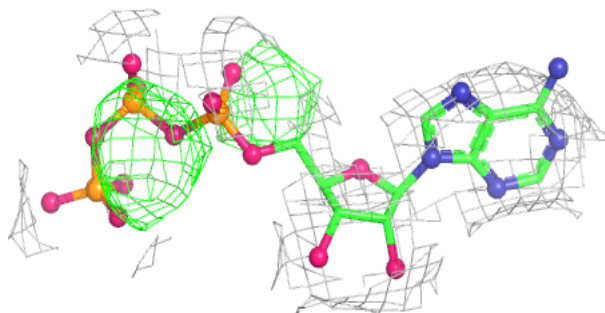
Electron density around LAR C 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

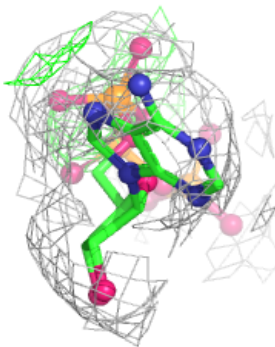
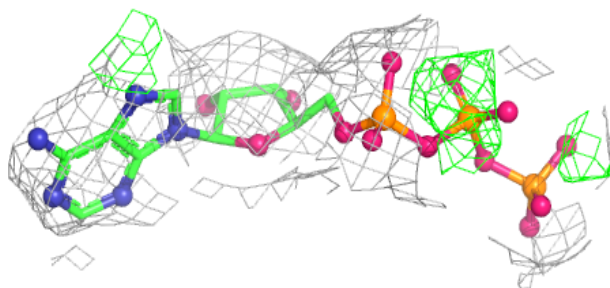
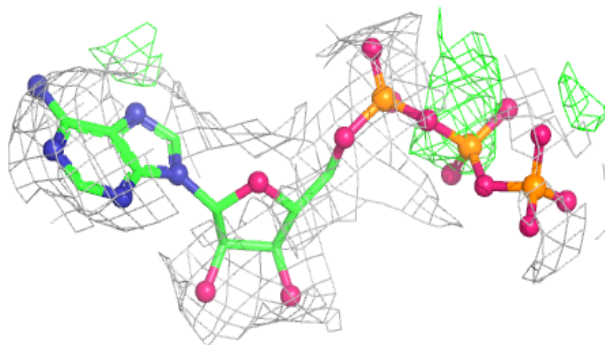


Electron density around ATP A 502:

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

**Electron density around ATP D 502:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.