



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:20 PM UTC

PDB ID : 3RUS / pdb_00003rus
Title : Crystal structure of Cpn-rls in complex with ADP from Methanococcus maripaludis
Authors : Pereira, J.H.; Ralston, C.Y.; Douglas, N.R.; Kumar, R.; McAndrew, R.P.; Knee, K.M.; King, J.A.; Frydman, J.; Adams, P.D.
Deposited on : 2011-05-05
Resolution : 2.34 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

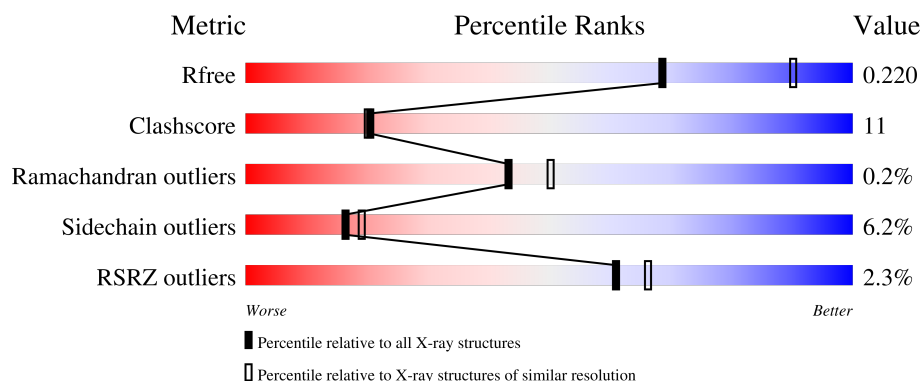
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	543	0% 70% 22% • 5%
1	B	543	3% 71% 22% • 5%
1	C	543	3% 75% 18% • 5%
1	D	543	2% 72% 21% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16140 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 Chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			3859	2397	666	771	25			
1	B	516	Total	C	N	O	S	0	0	0
			3859	2397	666	771	25			
1	C	516	Total	C	N	O	S	0	0	0
			3859	2397	666	771	25			
1	D	516	Total	C	N	O	S	0	0	0
			3859	2397	666	771	25			

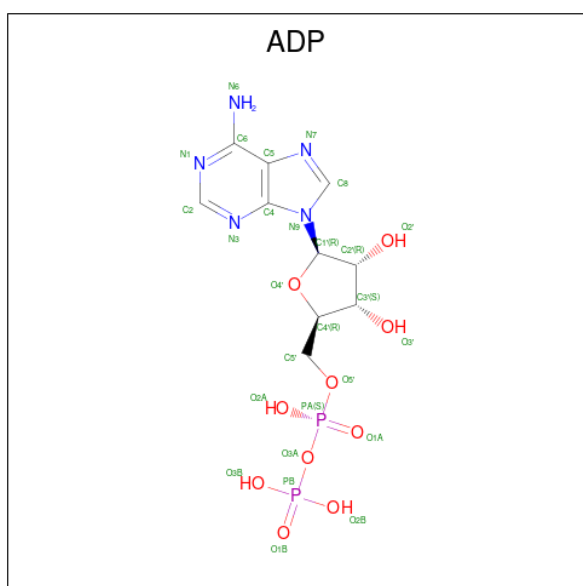
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ALA	THR	engineered mutation	UNP Q877G8
A	328	ALA	ASN	engineered mutation	UNP Q877G8
A	330	ALA	LYS	engineered mutation	UNP Q877G8
A	331	ALA	ASP	engineered mutation	UNP Q877G8
B	327	ALA	THR	engineered mutation	UNP Q877G8
B	328	ALA	ASN	engineered mutation	UNP Q877G8
B	330	ALA	LYS	engineered mutation	UNP Q877G8
B	331	ALA	ASP	engineered mutation	UNP Q877G8
C	327	ALA	THR	engineered mutation	UNP Q877G8
C	328	ALA	ASN	engineered mutation	UNP Q877G8
C	330	ALA	LYS	engineered mutation	UNP Q877G8
C	331	ALA	ASP	engineered mutation	UNP Q877G8
D	327	ALA	THR	engineered mutation	UNP Q877G8
D	328	ALA	ASN	engineered mutation	UNP Q877G8
D	330	ALA	LYS	engineered mutation	UNP Q877G8
D	331	ALA	ASP	engineered mutation	UNP Q877G8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

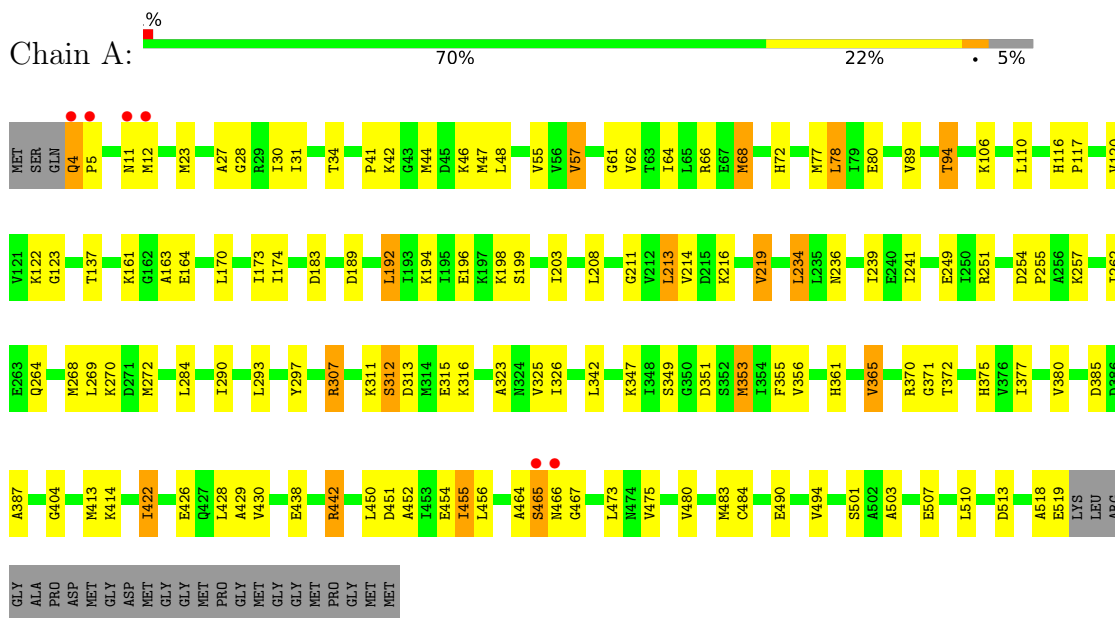
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		
5	B	128	Total	O	0	0
			128	128		
5	C	136	Total	O	0	0
			136	136		
5	D	125	Total	O	0	0
			125	125		

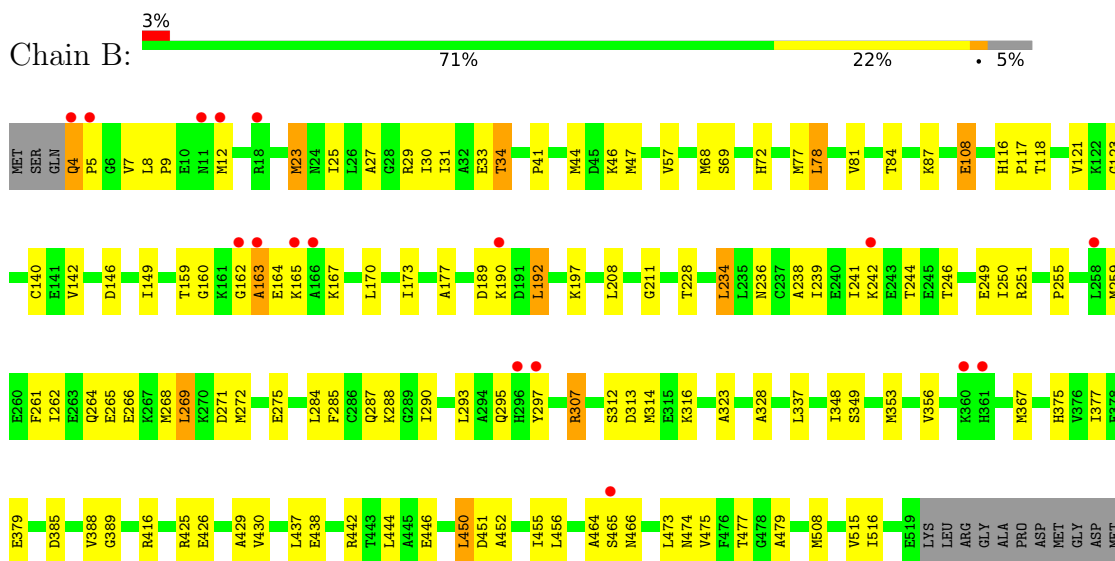
3 Residue-property plots

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: Chaperonin



• Molecule 1: Chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	161.56Å 185.59Å 185.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.34 49.04 – 2.34	Depositor EDS
% Data completeness (in resolution range)	93.5 (49.04-2.34) 99.8 (49.04-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.173 , 0.221 0.174 , 0.220	Depositor DCC
R_{free} test set	5866 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16140	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, 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	0.56	0/3883	0.85	2/5228 (0.0%)
1	B	0.52	0/3883	0.80	0/5228
1	C	0.53	0/3883	0.83	0/5228
1	D	0.50	0/3883	0.78	0/5228
All	All	0.53	0/15532	0.82	2/20912 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ALA	N-CA-C	-8.12	102.94	113.17
1	A	68	MET	N-CA-C	-7.00	100.83	110.35

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	3859	0	4001	107	0
1	B	3859	0	4001	107	0
1	C	3859	0	4001	90	0
1	D	3859	0	4001	99	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	4	0
3	B	27	0	12	0	0
3	C	27	0	12	2	0
3	D	27	0	12	1	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	163	0	0	3	0
5	B	128	0	0	1	0
5	C	136	0	0	4	0
5	D	125	0	0	3	0
All	All	16140	0	16052	353	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 11.

All (353) 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:C:161:LYS:O	5:C:553:HOH:O	1.91	0.87
1:B:477:THR:HG22	1:B:479:ALA:H	1.40	0.87
1:A:57:VAL:HG22	1:B:508:MET:HE2	1.57	0.87
1:D:141:GLU:HG2	1:D:399:ARG:HH11	1.39	0.87
1:A:61:GLY:HA3	1:A:94:THR:HG22	1.58	0.85
1:B:442:ARG:HG3	1:B:452:ALA:HB1	1.59	0.84
1:A:455:ILE:HG13	1:A:473:LEU:HD22	1.60	0.83
1:A:198:LYS:HE2	1:A:353:MET:HE1	1.60	0.83
1:C:44:MET:HE2	1:C:44:MET:HA	1.61	0.82
1:D:34:THR:O	1:D:46:LYS:HE3	1.80	0.82
1:D:442:ARG:HG3	1:D:452:ALA:HB1	1.61	0.81
1:C:234:LEU:HD22	1:C:323:ALA:HB3	1.64	0.80
1:C:161:LYS:HE3	5:C:678:HOH:O	1.80	0.80
1:B:287:GLN:HG3	1:B:314:MET:HG3	1.64	0.79
1:C:27:ALA:HA	1:D:7:VAL:HG21	1.65	0.79
1:B:313:ASP:HA	1:B:316:LYS:HE2	1.65	0.77
1:A:189:ASP:HB3	1:A:192:LEU:HD22	1.66	0.76
1:A:203:ILE:HD12	1:A:380:VAL:HG21	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASP:OD1	1:B:316:LYS:HE2	1.87	0.75
1:D:146:ASP:O	1:D:149:ILE:HG22	1.87	0.75
1:D:44:MET:HA	1:D:44:MET:HE2	1.69	0.74
3:A:545:ADP:O3B	5:A:567:HOH:O	2.04	0.74
1:A:68:MET:HE2	1:B:516:ILE:HD13	1.68	0.74
1:A:475:VAL:HG11	5:A:699:HOH:O	1.87	0.73
1:B:269:LEU:HD12	1:B:272:MET:HE2	1.70	0.73
1:A:313:ASP:HA	1:A:316:LYS:HE2	1.70	0.72
1:B:293:LEU:HD13	1:C:328:ALA:HB2	1.71	0.72
1:C:173:ILE:HG23	1:C:208:LEU:HB2	1.71	0.72
1:A:30:ILE:O	1:A:34:THR:HG23	1.90	0.71
1:D:28:GLY:HA2	1:D:78:LEU:HD22	1.72	0.71
1:D:209:ILE:HD13	1:D:213:LEU:HD11	1.73	0.71
1:C:442:ARG:HG2	1:C:442:ARG:HH11	1.54	0.71
1:C:241:ILE:HD11	1:C:265:GLU:O	1.91	0.70
1:D:141:GLU:HG2	1:D:399:ARG:NH1	2.07	0.70
1:D:161:LYS:HE3	5:D:667:HOH:O	1.91	0.70
1:A:349:SER:O	1:B:87:LYS:HE2	1.92	0.69
1:B:146:ASP:O	1:B:149:ILE:HG22	1.92	0.69
1:A:164:GLU:HG2	5:A:698:HOH:O	1.92	0.68
1:D:241:ILE:HD11	1:D:269:LEU:HD21	1.76	0.67
1:C:442:ARG:HG3	1:C:452:ALA:HB1	1.76	0.67
1:A:213:LEU:HD11	1:A:355:PHE:CD1	2.29	0.66
1:C:209:ILE:HD13	1:C:213:LEU:HD11	1.77	0.66
1:C:23:MET:HE3	1:C:72:HIS:NE2	2.11	0.66
1:D:249:GLU:HG2	1:D:251:ARG:HH12	1.61	0.66
1:B:450:LEU:HD23	1:B:473:LEU:HD21	1.78	0.65
1:C:27:ALA:HA	1:D:7:VAL:CG2	2.25	0.65
1:C:315:GLU:O	1:C:319:LYS:HG2	1.97	0.65
1:B:234:LEU:HD22	1:B:323:ALA:HB3	1.78	0.65
1:A:264:GLN:HG3	1:A:268:MET:HE3	1.78	0.64
1:B:30:ILE:O	1:B:34:THR:HG23	1.97	0.64
1:A:375:HIS:HB3	1:B:508:MET:HE1	1.78	0.64
1:C:23:MET:HE3	1:C:72:HIS:HE2	1.63	0.64
1:D:287:GLN:HE22	1:D:311:LYS:HE2	1.63	0.63
1:C:349:SER:HB3	1:D:87:LYS:NZ	2.14	0.63
1:B:190:LYS:HE2	1:B:389:GLY:HA2	1.79	0.63
1:B:189:ASP:HB3	1:B:192:LEU:HD22	1.81	0.62
1:C:293:LEU:HD13	1:D:328:ALA:HB2	1.81	0.62
1:C:216:LYS:HE2	1:C:307:ARG:O	2.00	0.62
1:A:44:MET:CE	1:B:118:THR:HG23	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:HG3	1:A:452:ALA:HB1	1.82	0.61
1:B:41:PRO:HG2	1:B:475:VAL:HG21	1.83	0.61
1:C:189:ASP:HB3	1:C:192:LEU:HD12	1.84	0.60
1:C:259:MET:SD	1:D:268:MET:HE3	2.41	0.60
1:C:442:ARG:HD3	1:C:456:LEU:HD22	1.83	0.60
1:D:116:HIS:CD2	1:D:118:THR:H	2.20	0.60
1:A:57:VAL:CG2	1:B:508:MET:HE2	2.31	0.60
1:B:241:ILE:HD11	1:B:265:GLU:O	2.02	0.60
1:B:27:ALA:HA	1:C:7:VAL:CG2	2.32	0.60
1:C:271:ASP:O	1:C:275:GLU:HG3	2.01	0.59
1:D:464:ALA:O	1:D:465:SER:HB3	2.03	0.59
1:B:197:LYS:HB3	1:B:377:ILE:HG21	1.85	0.58
1:B:442:ARG:HG3	1:B:452:ALA:CB	2.32	0.58
1:B:173:ILE:HG23	1:B:208:LEU:HB2	1.85	0.58
1:C:227:VAL:HG22	1:C:230:ALA:HB2	1.84	0.58
1:A:173:ILE:HG23	1:A:208:LEU:HB2	1.84	0.58
1:A:375:HIS:CE1	1:B:77:MET:HE1	2.38	0.58
1:A:451:ASP:HB3	1:A:454:GLU:HG2	1.85	0.58
1:B:164:GLU:O	1:B:167:LYS:HG2	2.03	0.58
1:D:185:GLU:CD	1:D:185:GLU:H	2.11	0.58
1:B:44:MET:HE2	1:B:44:MET:HA	1.86	0.58
1:C:86:GLU:HG2	5:C:676:HOH:O	2.04	0.58
1:D:213:LEU:HD23	1:D:353:MET:HE1	1.86	0.58
1:A:23:MET:HE3	1:A:72:HIS:CE1	2.39	0.58
1:D:116:HIS:HD2	1:D:118:THR:OG1	1.86	0.58
1:D:249:GLU:HG2	1:D:251:ARG:NH1	2.19	0.58
1:B:477:THR:HG22	1:B:479:ALA:N	2.14	0.57
1:D:465:SER:OG	1:D:466:ASN:N	2.37	0.57
1:A:464:ALA:O	1:A:465:SER:HB3	2.02	0.57
1:C:155:MET:CE	1:C:167:LYS:HE3	2.34	0.57
1:A:61:GLY:CA	1:A:94:THR:HG22	2.32	0.57
1:D:121:VAL:O	1:D:125:GLN:HG2	2.04	0.57
1:B:238:ALA:HB2	1:B:288:LYS:HB3	1.87	0.57
1:B:162:GLY:O	1:B:163:ALA:CB	2.53	0.57
1:A:44:MET:HE1	1:B:118:THR:HG23	1.87	0.57
1:B:27:ALA:HA	1:C:7:VAL:HG21	1.87	0.56
1:C:48:LEU:HD23	1:D:516:ILE:HB	1.85	0.56
1:B:9:PRO:HG2	1:B:12:MET:HE3	1.86	0.56
1:B:262:ILE:HD13	1:C:242:LYS:HB3	1.87	0.56
1:A:194:LYS:HE2	1:A:316:LYS:HD3	1.87	0.56
1:C:249:GLU:HG2	1:C:251:ARG:HH12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:CE	1:B:389:GLY:HA2	2.36	0.56
1:D:30:ILE:O	1:D:34:THR:HG22	2.05	0.56
1:B:78:LEU:O	1:B:81:VAL:HB	2.05	0.56
1:C:199:SER:HA	1:C:377:ILE:HD11	1.88	0.56
1:C:235:LEU:HD13	1:C:329:ILE:HD13	1.89	0.56
1:D:236:ASN:OD1	1:D:327:ALA:HA	2.06	0.55
1:B:262:ILE:HD11	1:C:242:LYS:O	2.07	0.55
1:B:140:CYS:SG	5:B:664:HOH:O	2.57	0.55
1:D:442:ARG:HG3	1:D:452:ALA:CB	2.35	0.55
1:C:47:MET:HE2	1:D:515:VAL:HG22	1.88	0.55
1:B:348:ILE:CG2	1:B:353:MET:HE2	2.37	0.55
1:A:422:ILE:HD12	1:A:430:VAL:HG21	1.89	0.55
1:D:34:THR:O	1:D:46:LYS:CE	2.53	0.55
1:D:199:SER:HA	1:D:377:ILE:HD11	1.88	0.54
1:A:251:ARG:NH1	1:B:249:GLU:HB2	2.23	0.54
1:B:464:ALA:O	1:B:465:SER:HB3	2.07	0.54
1:D:241:ILE:HD12	5:D:661:HOH:O	2.07	0.54
1:A:68:MET:HE2	1:B:516:ILE:CD1	2.36	0.54
1:A:214:VAL:O	1:A:353:MET:HG3	2.08	0.54
1:C:291:ASP:O	1:C:295:GLN:HG3	2.07	0.54
1:B:25:ILE:HD13	1:B:108:GLU:HB2	1.89	0.54
1:B:162:GLY:O	1:B:163:ALA:HB2	2.06	0.53
1:C:349:SER:HB3	1:D:87:LYS:HZ3	1.73	0.53
1:A:255:PRO:HA	1:B:261:PHE:CE1	2.43	0.53
1:A:270:LYS:HE2	1:A:297:TYR:OH	2.08	0.53
1:C:166:ALA:O	1:C:170:LEU:HB2	2.09	0.53
1:C:490:GLU:OE2	3:C:545:ADP:O2'	2.25	0.53
1:D:236:ASN:HA	1:D:287:GLN:HB3	1.90	0.53
1:A:450:LEU:CD1	1:A:473:LEU:HD21	2.39	0.53
1:B:234:LEU:HD12	1:B:285:PHE:HB2	1.91	0.53
1:C:277:LYS:HD3	1:C:301:GLU:HB3	1.89	0.53
1:B:269:LEU:HD12	1:B:272:MET:CE	2.36	0.53
1:C:293:LEU:HG	1:C:297:TYR:CE2	2.43	0.53
1:B:465:SER:OG	1:B:466:ASN:N	2.42	0.53
1:B:190:LYS:HE3	1:B:388:VAL:HG12	1.90	0.52
1:C:34:THR:O	1:C:46:LYS:HE3	2.09	0.52
1:D:173:ILE:HG23	1:D:208:LEU:HB2	1.91	0.52
1:B:46:LYS:HD2	1:C:514:ASP:HB3	1.91	0.52
1:C:238:ALA:HB2	1:C:288:LYS:HB3	1.91	0.52
1:B:312:SER:O	1:B:316:LYS:HG2	2.10	0.52
1:D:241:ILE:HD12	1:D:241:ILE:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:VAL:O	1:D:388:VAL:HG23	2.10	0.52
1:A:483:MET:HE2	1:A:483:MET:HA	1.91	0.52
1:A:313:ASP:OD1	1:A:316:LYS:HE2	2.10	0.52
1:A:44:MET:CE	1:B:116:HIS:CE1	2.93	0.51
1:A:311:LYS:O	1:A:315:GLU:HG3	2.10	0.51
1:D:116:HIS:CD2	1:D:118:THR:OG1	2.63	0.51
1:B:41:PRO:HB3	1:B:159:THR:HG22	1.93	0.51
1:D:201:ALA:HB3	1:D:205:ASP:OD2	2.11	0.51
1:A:4:GLN:HA	1:A:4:GLN:OE1	2.09	0.51
1:A:44:MET:HE3	1:B:116:HIS:CE1	2.46	0.51
1:B:290:ILE:HD12	1:B:307:ARG:HB3	1.92	0.51
1:B:47:MET:HE2	1:C:515:VAL:HG22	1.92	0.51
1:A:293:LEU:HD13	1:B:328:ALA:HB2	1.93	0.50
1:C:155:MET:HE2	1:C:167:LYS:HE3	1.93	0.50
1:A:11:ASN:OD1	1:A:519:GLU:HA	2.11	0.50
1:D:241:ILE:CD1	1:D:269:LEU:HD21	2.41	0.50
1:D:293:LEU:HG	1:D:297:TYR:CE2	2.47	0.50
1:A:465:SER:OG	1:A:466:ASN:N	2.44	0.50
1:C:293:LEU:CD1	1:D:328:ALA:HB2	2.41	0.50
1:D:239:ILE:HD11	1:D:284:LEU:HD21	1.94	0.50
1:D:412:SER:HB2	1:D:434:ALA:O	2.12	0.50
1:A:34:THR:O	1:A:46:LYS:HE3	2.11	0.50
1:A:219:VAL:HG23	1:A:307:ARG:HG2	1.93	0.50
1:D:65:LEU:HB3	1:D:79:ILE:HD12	1.92	0.50
1:A:264:GLN:O	1:A:268:MET:HG3	2.11	0.50
1:D:412:SER:O	1:D:416:ARG:HG3	2.12	0.50
1:A:48:LEU:HD23	1:B:516:ILE:HB	1.94	0.50
1:A:264:GLN:NE2	1:A:264:GLN:HA	2.27	0.49
1:B:416:ARG:HH22	1:B:438:GLU:CD	2.19	0.49
1:B:455:ILE:HD12	1:B:455:ILE:C	2.36	0.49
1:D:234:LEU:HD22	1:D:314:MET:HE1	1.94	0.49
1:B:123:GLY:HA3	1:B:429:ALA:HB3	1.94	0.49
1:B:271:ASP:O	1:B:275:GLU:HG3	2.12	0.49
1:C:174:ILE:HD13	1:C:387:ALA:HB3	1.95	0.49
1:A:27:ALA:HA	1:B:7:VAL:HG21	1.95	0.49
1:C:442:ARG:HG2	1:C:442:ARG:NH1	2.27	0.49
1:D:313:ASP:OD1	1:D:316:LYS:HE2	2.13	0.49
1:A:44:MET:HE2	1:B:118:THR:HG23	1.95	0.49
1:D:404:GLY:HA2	3:D:545:ADP:N3	2.28	0.49
1:C:307:ARG:HD3	1:C:308:ARG:HG3	1.95	0.48
1:B:236:ASN:HA	1:B:287:GLN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:VAL:HG11	1:C:316:LYS:HB3	1.96	0.48
1:C:249:GLU:HG2	1:C:251:ARG:NH1	2.28	0.48
1:D:196:GLU:HG3	1:D:213:LEU:HD22	1.95	0.48
1:D:234:LEU:HD22	1:D:314:MET:CE	2.43	0.48
1:A:110:LEU:HD21	1:A:429:ALA:HA	1.94	0.48
1:D:227:VAL:HG22	1:D:230:ALA:HB2	1.95	0.48
1:D:291:ASP:O	1:D:295:GLN:HG3	2.14	0.48
1:B:165:LYS:HD3	1:C:125:GLN:HB3	1.95	0.48
1:C:264:GLN:HA	1:C:264:GLN:NE2	2.29	0.48
1:C:490:GLU:HG2	5:C:615:HOH:O	2.14	0.48
1:D:211:GLY:HA3	1:D:356:VAL:O	2.14	0.48
1:A:208:LEU:HD11	1:A:365:VAL:HG13	1.96	0.47
1:C:459:VAL:O	1:C:463:HIS:HD2	1.96	0.47
1:C:490:GLU:OE1	1:C:495:LYS:HE2	2.15	0.47
1:A:62:VAL:O	1:A:66:ARG:HG3	2.14	0.47
1:C:284:LEU:O	1:C:305:ALA:HA	2.14	0.47
1:D:197:LYS:HB3	1:D:377:ILE:HG21	1.96	0.47
1:D:174:ILE:HD13	1:D:387:ALA:HB3	1.97	0.47
1:B:348:ILE:HG21	1:B:353:MET:HE2	1.96	0.47
1:D:22:ARG:O	1:D:26:LEU:HB2	2.15	0.47
1:D:252:ILE:HD13	1:D:258:LEU:HD23	1.96	0.47
1:D:348:ILE:HG21	1:D:353:MET:HE2	1.96	0.47
1:B:259:MET:CE	1:C:268:MET:HE2	2.45	0.47
1:C:29:ARG:O	1:C:33:GLU:HG3	2.15	0.47
1:D:367:MET:HB3	1:D:367:MET:HE2	1.67	0.47
1:C:4:GLN:HA	1:C:5:PRO:HA	1.79	0.47
1:C:404:GLY:HA2	3:C:545:ADP:N3	2.30	0.47
1:D:27:ALA:HB2	1:D:72:HIS:CE1	2.50	0.47
1:A:442:ARG:CG	1:A:452:ALA:HB1	2.45	0.46
1:B:313:ASP:OD1	1:B:316:LYS:CE	2.60	0.46
1:D:284:LEU:O	1:D:305:ALA:HA	2.15	0.46
1:C:442:ARG:HH11	1:C:442:ARG:CG	2.25	0.46
1:A:174:ILE:HD13	1:A:387:ALA:HB3	1.97	0.46
1:A:466:ASN:HA	1:A:467:GLY:HA3	1.73	0.46
1:B:295:GLN:HE22	1:B:307:ARG:HH21	1.64	0.46
1:C:13:LYS:HD2	1:C:13:LYS:N	2.31	0.46
1:B:426:GLU:O	1:B:430:VAL:HG23	2.16	0.46
1:D:4:GLN:N	1:D:5:PRO:CD	2.79	0.46
1:A:211:GLY:HA3	1:A:356:VAL:O	2.15	0.46
1:A:213:LEU:HD11	1:A:355:PHE:CE1	2.51	0.46
1:A:239:ILE:HD12	1:A:290:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:PRO:HA	1:C:261:PHE:CE2	2.51	0.46
1:C:44:MET:HA	1:C:44:MET:CE	2.40	0.46
1:C:164:GLU:O	1:C:167:LYS:HB2	2.16	0.46
1:D:184:ASP:HA	1:D:185:GLU:HA	1.67	0.45
1:A:208:LEU:HD11	1:A:365:VAL:CG1	2.47	0.45
1:A:161:LYS:O	1:A:164:GLU:HB2	2.16	0.45
1:A:47:MET:HE2	1:B:515:VAL:HG13	1.99	0.45
1:A:347:LYS:HA	1:A:351:ASP:O	2.17	0.45
1:D:238:ALA:HB2	1:D:288:LYS:CB	2.46	0.45
1:A:270:LYS:HE2	1:A:297:TYR:CZ	2.51	0.45
1:C:161:LYS:HA	1:C:161:LYS:HD3	1.70	0.45
1:C:372:THR:O	1:D:84:THR:HG21	2.16	0.45
1:A:77:MET:O	1:A:80:GLU:HG2	2.17	0.45
1:C:236:ASN:O	1:C:288:LYS:HD3	2.16	0.45
1:D:273:VAL:HG21	1:D:297:TYR:HB2	1.99	0.45
1:D:409:VAL:HG11	1:D:459:VAL:HG12	1.99	0.45
1:D:177:ALA:HB2	1:D:208:LEU:HD13	1.98	0.45
1:D:203:ILE:HA	1:D:370:ARG:O	2.17	0.45
1:A:123:GLY:HA3	1:A:429:ALA:HB3	1.98	0.45
1:A:219:VAL:CG2	1:A:307:ARG:HG2	2.47	0.45
1:C:219:VAL:HG12	1:C:223:MET:HE1	1.98	0.45
1:A:183:ASP:OD1	1:A:183:ASP:C	2.60	0.44
1:D:268:MET:HE2	5:D:662:HOH:O	2.15	0.44
1:A:41:PRO:HG3	3:A:545:ADP:C5	2.52	0.44
1:D:28:GLY:CA	1:D:78:LEU:HD22	2.45	0.44
1:D:185:GLU:CD	1:D:185:GLU:N	2.76	0.44
1:A:262:ILE:HD13	1:B:242:LYS:HB3	1.98	0.44
1:A:312:SER:O	1:A:316:LYS:HG2	2.18	0.44
1:C:411:LEU:HD12	1:C:411:LEU:HA	1.85	0.44
1:B:211:GLY:HA3	1:B:356:VAL:O	2.18	0.44
1:C:455:ILE:O	1:C:459:VAL:HG23	2.18	0.44
1:D:116:HIS:HD2	1:D:118:THR:H	1.66	0.44
1:A:234:LEU:HD22	1:A:323:ALA:HB3	2.00	0.44
1:A:254:ASP:HA	1:A:255:PRO:HD2	1.87	0.44
1:B:69:SER:O	1:C:9:PRO:HG3	2.18	0.44
1:D:30:ILE:O	1:D:34:THR:CG2	2.66	0.44
1:C:201:ALA:O	1:D:500:GLN:HG2	2.18	0.44
1:D:123:GLY:HA3	1:D:429:ALA:HB3	1.98	0.44
1:A:442:ARG:HG2	1:A:442:ARG:HH11	1.82	0.43
1:A:503:ALA:O	1:A:507:GLU:HG3	2.18	0.43
1:C:442:ARG:NH1	1:C:442:ARG:CG	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASN:HB2	1:A:325:VAL:HG12	1.99	0.43
1:B:23:MET:HE3	1:B:72:HIS:CE1	2.53	0.43
1:A:213:LEU:HD12	1:A:213:LEU:HA	1.78	0.43
1:B:177:ALA:HB2	1:B:208:LEU:HD13	2.01	0.43
1:D:425:ARG:HG2	1:D:425:ARG:HH11	1.83	0.43
1:B:249:GLU:HB3	1:B:251:ARG:NH1	2.33	0.43
1:D:195:ILE:HG23	1:D:369:ILE:HD12	2.00	0.43
1:B:379:GLU:OE2	1:B:379:GLU:HA	2.19	0.43
1:C:197:LYS:O	1:C:198:LYS:HD2	2.18	0.43
1:D:268:MET:O	1:D:272:MET:HG3	2.18	0.43
1:B:239:ILE:HD11	1:B:284:LEU:HD21	2.00	0.43
1:A:196:GLU:HG2	1:A:213:LEU:HD23	2.00	0.43
1:B:29:ARG:O	1:B:33:GLU:HG3	2.19	0.43
1:D:314:MET:HA	1:D:314:MET:HE2	2.01	0.43
1:A:199:SER:HA	1:A:377:ILE:HD11	2.01	0.43
1:A:513:ASP:OD1	1:A:513:ASP:C	2.61	0.43
1:A:116:HIS:CD2	1:A:117:PRO:HD2	2.54	0.42
1:A:438:GLU:O	1:A:442:ARG:HB2	2.18	0.42
1:D:149:ILE:HD12	1:D:149:ILE:HA	1.84	0.42
1:A:4:GLN:N	1:A:5:PRO:HD2	2.34	0.42
1:B:30:ILE:HD12	1:C:7:VAL:HG21	2.01	0.42
1:D:31:ILE:HD13	1:D:31:ILE:HA	1.78	0.42
1:A:404:GLY:HA2	3:A:545:ADP:N3	2.34	0.42
1:C:451:ASP:OD2	1:C:454:GLU:HG2	2.20	0.42
1:D:178:VAL:HG13	1:D:188:VAL:HG11	2.01	0.42
1:C:464:ALA:O	1:C:465:SER:HB2	2.18	0.42
1:A:89:VAL:HG11	1:A:494:VAL:HG22	2.02	0.42
1:A:64:ILE:CG2	1:A:68:MET:HE3	2.50	0.42
1:A:216:LYS:HE3	1:A:307:ARG:O	2.19	0.42
1:A:251:ARG:HD2	1:B:251:ARG:HG2	2.01	0.42
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.87	0.42
1:A:94:THR:HG23	3:A:545:ADP:O3B	2.20	0.42
1:A:116:HIS:CG	1:A:117:PRO:HD2	2.55	0.42
1:D:194:LYS:HE2	1:D:316:LYS:HD3	2.02	0.42
1:A:27:ALA:HA	1:B:7:VAL:CG2	2.50	0.42
1:B:9:PRO:HG2	1:B:12:MET:CE	2.50	0.42
1:B:269:LEU:HD12	1:B:269:LEU:HA	1.83	0.42
1:B:287:GLN:HG3	1:B:314:MET:CG	2.42	0.42
1:C:63:THR:O	1:C:67:GLU:HG2	2.20	0.42
1:C:69:SER:O	1:D:9:PRO:HG3	2.20	0.42
1:D:201:ALA:O	1:D:202:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HE2	1:A:316:LYS:CD	2.49	0.41
1:A:203:ILE:HD13	1:A:371:GLY:HA2	2.02	0.41
1:A:262:ILE:HD11	1:B:242:LYS:O	2.20	0.41
1:B:474:ASN:OD1	1:B:477:THR:HB	2.20	0.41
1:D:178:VAL:HA	1:D:193:ILE:HD11	2.02	0.41
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.88	0.41
1:B:367:MET:HE3	1:B:367:MET:HB3	1.79	0.41
1:C:455:ILE:C	1:C:455:ILE:HD12	2.45	0.41
1:A:249:GLU:HG2	1:A:251:ARG:HH12	1.85	0.41
1:A:293:LEU:HD12	1:A:293:LEU:O	2.21	0.41
1:B:41:PRO:HA	1:B:160:GLY:HA3	2.02	0.41
1:B:293:LEU:HG	1:B:297:TYR:CE2	2.54	0.41
1:A:27:ALA:HB2	1:A:72:HIS:CE1	2.55	0.41
1:D:62:VAL:O	1:D:66:ARG:HG3	2.21	0.41
1:D:103:LEU:HD23	1:D:103:LEU:HA	1.91	0.41
1:D:293:LEU:HD12	1:D:293:LEU:HA	1.83	0.41
1:D:408:GLU:OE2	1:D:495:LYS:NZ	2.51	0.41
1:B:116:HIS:CG	1:B:117:PRO:HD2	2.56	0.41
1:A:413:MET:CE	1:A:414:LYS:NZ	2.84	0.41
1:A:518:ALA:O	1:A:519:GLU:C	2.64	0.41
1:A:198:LYS:O	1:A:370:ARG:HA	2.21	0.41
1:A:372:THR:O	1:B:84:THR:HG21	2.21	0.41
1:A:450:LEU:HD12	1:A:473:LEU:HD21	2.03	0.41
1:B:266:GLU:OE1	1:C:242:LYS:NZ	2.54	0.41
1:B:348:ILE:O	1:B:349:SER:HB2	2.21	0.41
1:C:273:VAL:HG21	1:C:297:TYR:HB2	2.03	0.41
1:D:116:HIS:CG	1:D:117:PRO:HD2	2.56	0.41
1:C:349:SER:HB3	1:D:87:LYS:HZ1	1.83	0.41
1:A:257:LYS:HA	1:A:257:LYS:HD3	1.87	0.40
1:A:455:ILE:HG13	1:A:473:LEU:CD2	2.42	0.40
1:B:4:GLN:HA	1:B:5:PRO:HD3	1.91	0.40
1:B:284:LEU:HD12	1:B:285:PHE:N	2.36	0.40
1:D:264:GLN:O	1:D:268:MET:HG3	2.21	0.40
1:A:122:LYS:HD3	1:A:426:GLU:OE1	2.20	0.40
1:B:349:SER:O	1:C:87:LYS:HE2	2.21	0.40
1:B:375:HIS:ND1	1:C:80:GLU:OE2	2.51	0.40
1:D:12:MET:O	1:D:12:MET:HG2	2.21	0.40
1:D:209:ILE:CD1	1:D:213:LEU:HD11	2.47	0.40
1:B:197:LYS:HB3	1:B:377:ILE:CG2	2.51	0.40
1:B:264:GLN:O	1:B:268:MET:HG3	2.20	0.40
1:B:442:ARG:O	1:B:446:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ILE:HD12	1:D:290:ILE:HG12	2.03	0.40
1:A:28:GLY:HA2	1:A:78:LEU:HD21	2.02	0.40
1:A:268:MET:O	1:A:272:MET:HG3	2.22	0.40
1:B:451:ASP:O	1:B:455:ILE:HG23	2.20	0.40
1:C:116:HIS:CG	1:C:117:PRO:HD2	2.56	0.40
1:C:169:LYS:H	1:C:169:LYS:HG2	1.55	0.40
1:C:490:GLU:OE1	1:C:495:LYS:CE	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/543 (95%)	505 (98%)	8 (2%)	1 (0%)	43	50
1	B	514/543 (95%)	496 (96%)	17 (3%)	1 (0%)	43	50
1	C	514/543 (95%)	502 (98%)	10 (2%)	2 (0%)	30	32
1	D	514/543 (95%)	501 (98%)	13 (2%)	0	100	100
All	All	2056/2172 (95%)	2004 (98%)	48 (2%)	4 (0%)	43	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	ALA
1	C	465	SER
1	C	5	PRO
1	A	465	SER

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	412/430 (96%)	376 (91%)	36 (9%)	9	10
1	B	412/430 (96%)	386 (94%)	26 (6%)	16	19
1	C	412/430 (96%)	395 (96%)	17 (4%)	27	35
1	D	412/430 (96%)	389 (94%)	23 (6%)	19	23
All	All	1648/1720 (96%)	1546 (94%)	102 (6%)	16	19

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	12	MET
1	A	31	ILE
1	A	42	LYS
1	A	55	VAL
1	A	57	VAL
1	A	78	LEU
1	A	94	THR
1	A	106	LYS
1	A	120	VAL
1	A	137	THR
1	A	170	LEU
1	A	192	LEU
1	A	213	LEU
1	A	219	VAL
1	A	234	LEU
1	A	269	LEU
1	A	284	LEU
1	A	307	ARG
1	A	312	SER
1	A	326	ILE
1	A	342	LEU
1	A	353	MET
1	A	361	HIS

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Mol	Chain	Res	Type
1	A	365	VAL
1	A	385	ASP
1	A	422	ILE
1	A	428	LEU
1	A	442	ARG
1	A	455	ILE
1	A	456	LEU
1	A	480	VAL
1	A	484	CYS
1	A	490	GLU
1	A	501	SER
1	A	510	LEU
1	B	4	GLN
1	B	8	LEU
1	B	23	MET
1	B	31	ILE
1	B	34	THR
1	B	57	VAL
1	B	68	MET
1	B	78	LEU
1	B	108	GLU
1	B	121	VAL
1	B	142	VAL
1	B	192	LEU
1	B	228	THR
1	B	234	LEU
1	B	244	THR
1	B	246	THR
1	B	250	ILE
1	B	269	LEU
1	B	307	ARG
1	B	337	LEU
1	B	385	ASP
1	B	425	ARG
1	B	437	LEU
1	B	444	LEU
1	B	450	LEU
1	B	456	LEU
1	C	4	GLN
1	C	12	MET
1	C	52	LEU
1	C	55	VAL

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Mol	Chain	Res	Type
1	C	169	LYS
1	C	170	LEU
1	C	227	VAL
1	C	234	LEU
1	C	307	ARG
1	C	312	SER
1	C	329	ILE
1	C	339	ASP
1	C	361	HIS
1	C	425	ARG
1	C	428	LEU
1	C	442	ARG
1	C	484	CYS
1	D	8	LEU
1	D	12	MET
1	D	26	LEU
1	D	31	ILE
1	D	34	THR
1	D	78	LEU
1	D	106	LYS
1	D	111	LEU
1	D	185	GLU
1	D	227	VAL
1	D	244	THR
1	D	246	THR
1	D	269	LEU
1	D	312	SER
1	D	314	MET
1	D	319	LYS
1	D	339	ASP
1	D	348	ILE
1	D	352	SER
1	D	367	MET
1	D	456	LEU
1	D	484	CYS
1	D	495	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	497	GLN

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Mol	Chain	Res	Type
1	A	500	GLN
1	B	264	GLN
1	B	295	GLN
1	B	296	HIS
1	B	427	GLN
1	B	500	GLN
1	C	11	ASN
1	C	129	GLN
1	C	222	GLN
1	C	264	GLN
1	C	287	GLN
1	C	427	GLN
1	C	500	GLN
1	D	59	ASN
1	D	116	HIS
1	D	264	GLN
1	D	287	GLN
1	D	296	HIS
1	D	427	GLN
1	D	500	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
3	ADP	C	545	2	28,29,29	1.52	5 (17%)	43,45,45	1.85	10 (23%)
4	SO4	B	546	-	4,4,4	0.26	0	6,6,6	0.13	0
3	ADP	D	545	2	28,29,29	1.35	4 (14%)	43,45,45	1.83	9 (20%)
4	SO4	B	547	-	4,4,4	0.25	0	6,6,6	0.16	0
4	SO4	C	547	-	4,4,4	0.23	0	6,6,6	0.15	0
3	ADP	A	545	2	28,29,29	1.46	6 (21%)	43,45,45	1.84	11 (25%)
4	SO4	A	547	-	4,4,4	0.22	0	6,6,6	0.10	0
4	SO4	C	546	-	4,4,4	0.22	0	6,6,6	0.14	0
4	SO4	D	546	-	4,4,4	0.23	0	6,6,6	0.20	0
4	SO4	D	547	-	4,4,4	0.25	0	6,6,6	0.08	0
3	ADP	B	545	2	28,29,29	1.47	5 (17%)	43,45,45	1.82	9 (20%)
4	SO4	A	546	-	4,4,4	0.26	0	6,6,6	0.15	0

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	D	545	2	-	6/16/32/32	0/3/3/3
3	ADP	C	545	2	-	1/16/32/32	0/3/3/3
3	ADP	B	545	2	-	2/16/32/32	0/3/3/3
3	ADP	A	545	2	-	3/16/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	545	ADP	C5-C4	4.61	1.47	1.39
3	B	545	ADP	C5-C4	4.54	1.47	1.39
3	D	545	ADP	C5-C4	4.40	1.46	1.39
3	A	545	ADP	C5-C4	4.27	1.46	1.39
3	C	545	ADP	PA-O3A	3.25	1.63	1.59
3	A	545	ADP	PA-O3A	2.98	1.62	1.59
3	B	545	ADP	PA-O3A	2.87	1.62	1.59
3	B	545	ADP	C8-N7	2.74	1.36	1.31
3	B	545	ADP	C5-C6	2.68	1.48	1.41
3	C	545	ADP	C8-N7	2.67	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	545	ADP	C5-C6	2.65	1.48	1.41
3	B	545	ADP	C5-N7	-2.48	1.34	1.39
3	A	545	ADP	C5-C6	2.46	1.47	1.41
3	A	545	ADP	C5-N7	-2.46	1.34	1.39
3	D	545	ADP	C5-C6	2.44	1.47	1.41
3	C	545	ADP	C5-N7	-2.27	1.34	1.39
3	A	545	ADP	C4-N9	-2.21	1.33	1.37
3	D	545	ADP	C5-N7	-2.20	1.35	1.39
3	D	545	ADP	C8-N7	2.19	1.35	1.31
3	A	545	ADP	C8-N7	2.19	1.35	1.31

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	545	ADP	C5-C4-N3	-6.19	118.19	126.72
3	C	545	ADP	C5-C4-N3	-5.56	119.07	126.72
3	D	545	ADP	C5-C4-N3	-5.55	119.08	126.72
3	A	545	ADP	C5-C4-N3	-5.42	119.25	126.72
3	D	545	ADP	N3-C4-N9	4.97	135.62	127.17
3	B	545	ADP	N3-C4-N9	4.49	134.81	127.17
3	A	545	ADP	N3-C4-N9	4.40	134.65	127.17
3	C	545	ADP	N3-C4-N9	4.32	134.51	127.17
3	B	545	ADP	C2-N3-C4	3.89	121.32	111.83
3	B	545	ADP	C4-C5-N7	-3.69	106.37	110.58
3	C	545	ADP	C2-N3-C4	3.62	120.68	111.83
3	A	545	ADP	C2-N3-C4	3.62	120.67	111.83
3	C	545	ADP	O4'-C1'-N9	3.60	115.01	108.09
3	D	545	ADP	C2-N3-C4	3.57	120.54	111.83
3	A	545	ADP	N3-C2-N1	-3.52	123.25	128.58
3	D	545	ADP	C4-N9-C8	3.41	109.32	105.74
3	C	545	ADP	C4-C5-N7	-3.41	106.68	110.58
3	A	545	ADP	O4'-C1'-N9	3.40	114.62	108.09
3	A	545	ADP	C4-C5-N7	-3.27	106.84	110.58
3	C	545	ADP	N3-C2-N1	-3.18	123.77	128.58
3	D	545	ADP	N3-C2-N1	-3.14	123.83	128.58
3	B	545	ADP	N3-C2-N1	-3.13	123.84	128.58
3	A	545	ADP	C4-N9-C8	3.09	108.98	105.74
3	C	545	ADP	C4-N9-C8	2.80	108.68	105.74
3	D	545	ADP	C4-C5-N7	-2.67	107.53	110.58
3	B	545	ADP	C5-N7-C8	2.58	107.50	103.45
3	C	545	ADP	C5-N7-C8	2.51	107.40	103.45
3	A	545	ADP	C5-N7-C8	2.50	107.38	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	545	ADP	C5-N7-C8	2.31	107.07	103.45
3	C	545	ADP	C6-C5-N7	2.29	136.51	132.09
3	D	545	ADP	N6-C6-N1	2.28	123.45	118.38
3	A	545	ADP	N9-C8-N7	-2.27	110.71	113.94
3	B	545	ADP	O4'-C1'-N9	2.24	112.39	108.09
3	D	545	ADP	N9-C8-N7	-2.23	110.78	113.94
3	C	545	ADP	N9-C8-N7	-2.19	110.82	113.94
3	A	545	ADP	C2-N1-C6	2.18	122.32	118.73
3	B	545	ADP	C6-C5-N7	2.14	136.21	132.09
3	A	545	ADP	C6-C5-N7	2.14	136.21	132.09
3	B	545	ADP	C4-N9-C8	2.09	107.93	105.74

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	545	ADP	C5'-O5'-PA-O1A
3	D	545	ADP	PA-O3A-PB-O1B
3	A	545	ADP	C5'-O5'-PA-O1A
3	D	545	ADP	C5'-O5'-PA-O2A
3	D	545	ADP	C5'-O5'-PA-O3A
3	B	545	ADP	PB-O3A-PA-O1A
3	D	545	ADP	PA-O3A-PB-O2B
3	D	545	ADP	PA-O3A-PB-O3B
3	A	545	ADP	PB-O3A-PA-O1A
3	B	545	ADP	PB-O3A-PA-O2A
3	A	545	ADP	PB-O3A-PA-O2A
3	C	545	ADP	PB-O3A-PA-O2A

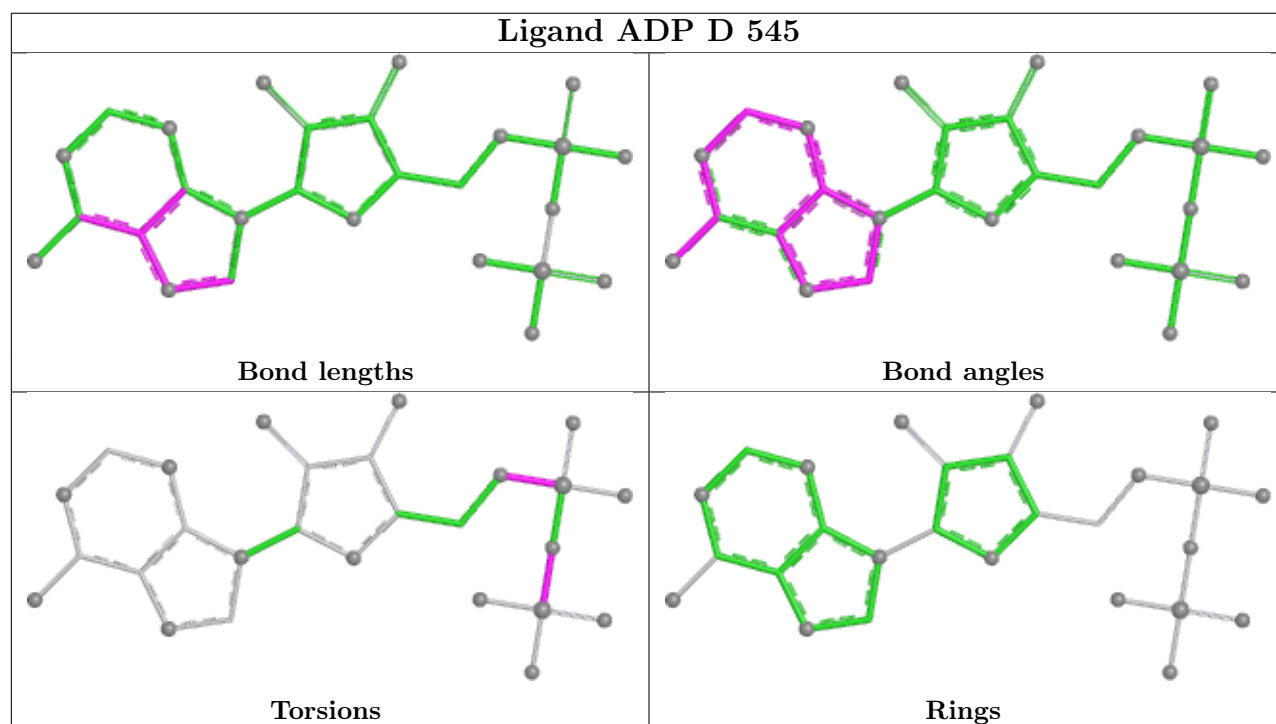
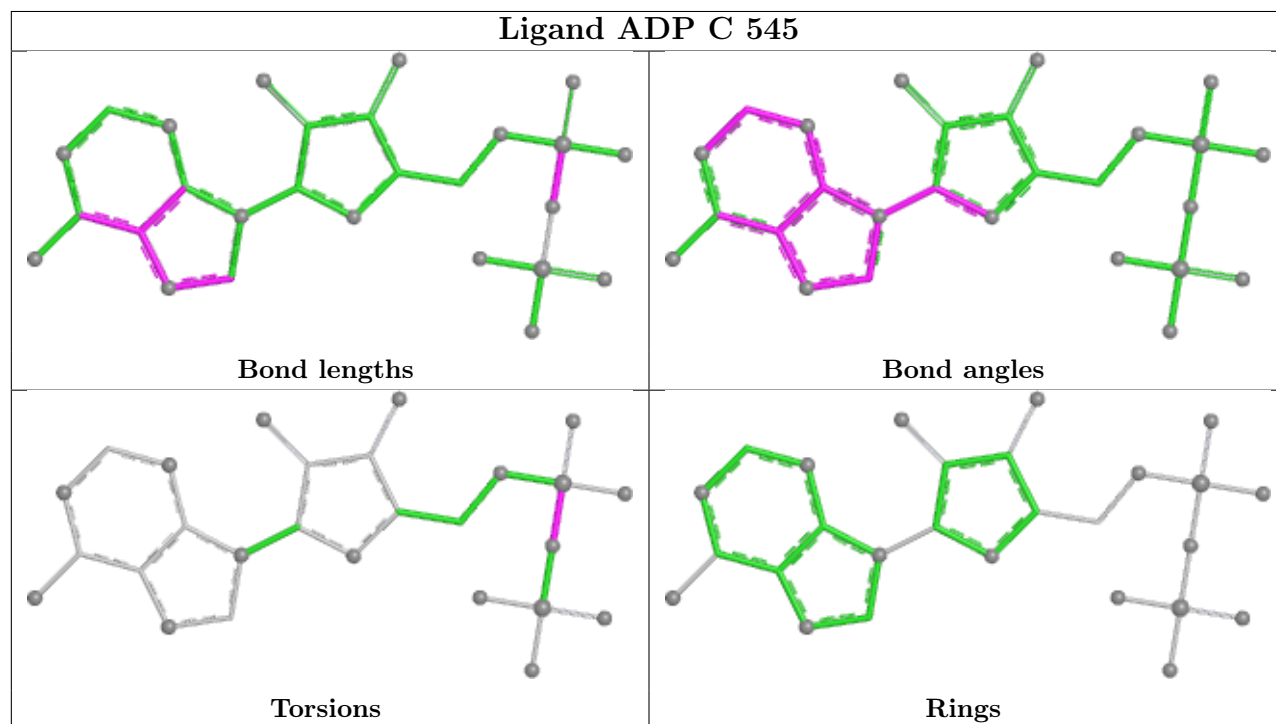
There are no ring outliers.

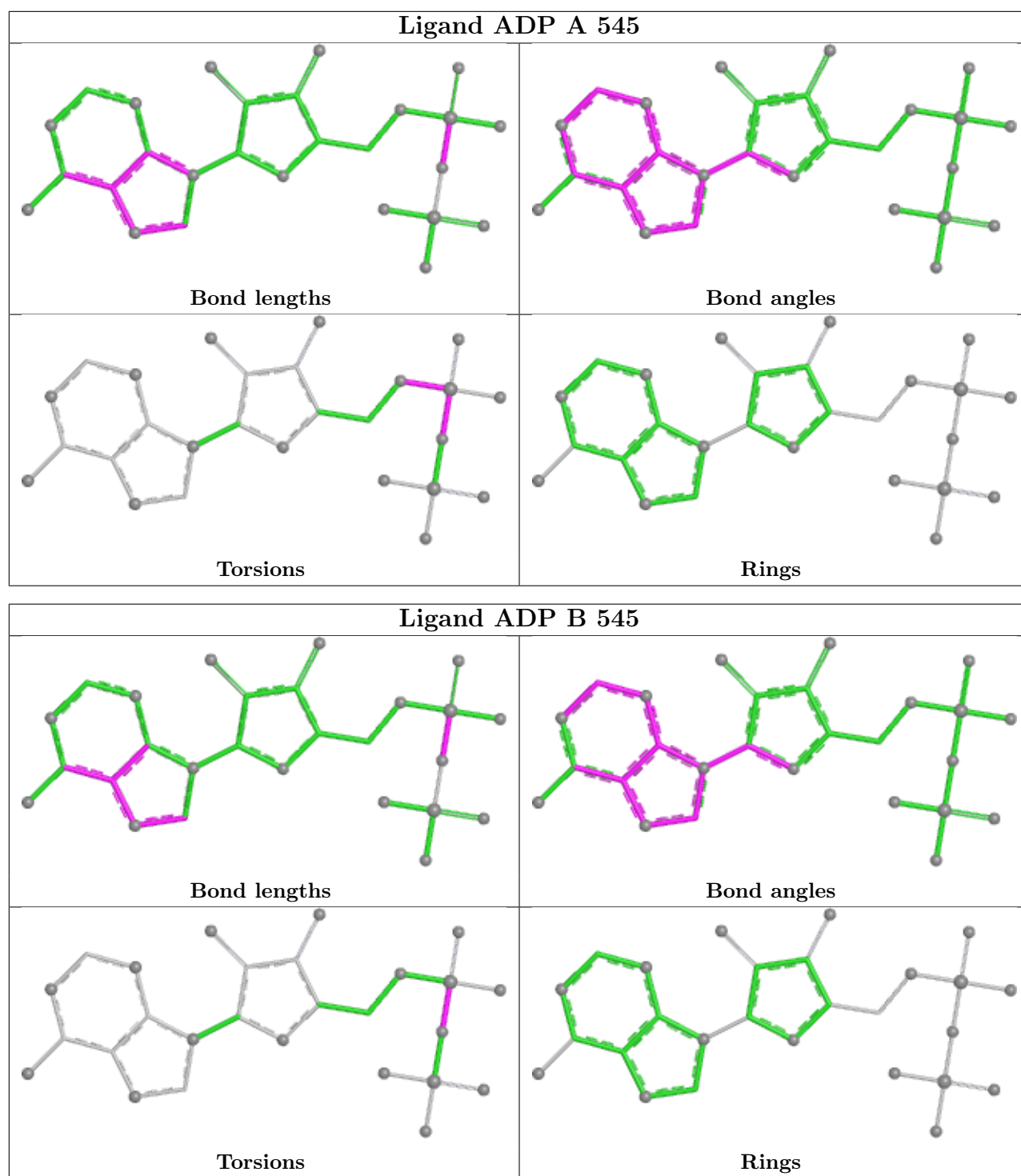
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	545	ADP	2	0
3	D	545	ADP	1	0
3	A	545	ADP	4	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 ⓘ

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(Å ²)	Q<0.9
1	A	516/543 (95%)	-0.21	6 (1%) 76 80	21, 48, 81, 119	0
1	B	516/543 (95%)	-0.05	17 (3%) 49 55	25, 50, 86, 127	0
1	C	516/543 (95%)	-0.07	15 (2%) 53 60	22, 51, 89, 125	0
1	D	516/543 (95%)	-0.07	10 (1%) 66 71	27, 55, 86, 137	0
All	All	2064/2172 (95%)	-0.10	48 (2%) 61 66	21, 51, 86, 137	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	SER	4.0
1	B	162	GLY	3.7
1	C	8	LEU	3.6
1	C	236	ASN	3.3
1	D	4	GLN	3.1
1	C	465	SER	3.1
1	C	163	ALA	3.1
1	B	163	ALA	3.0
1	B	18	ARG	3.0
1	C	69	SER	3.0
1	C	5	PRO	3.0
1	B	4	GLN	2.9
1	A	466	ASN	2.9
1	B	361	HIS	2.9
1	D	467	GLY	2.9
1	C	7	VAL	2.9
1	D	5	PRO	2.7
1	D	6	GLY	2.7
1	C	4	GLN	2.6
1	C	242	LYS	2.6
1	B	12	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	12	MET	2.5
1	B	5	PRO	2.5
1	A	11	ASN	2.4
1	B	360	LYS	2.4
1	A	5	PRO	2.4
1	C	162	GLY	2.4
1	D	11	ASN	2.3
1	B	165	LYS	2.3
1	D	297	TYR	2.3
1	C	519	GLU	2.3
1	C	466	ASN	2.3
1	D	162	GLY	2.3
1	C	327	ALA	2.2
1	A	4	GLN	2.2
1	B	166	ALA	2.2
1	B	465	SER	2.2
1	B	258	LEU	2.2
1	A	12	MET	2.1
1	B	297	TYR	2.1
1	C	361	HIS	2.1
1	D	256	ALA	2.1
1	B	242	LYS	2.0
1	D	184	ASP	2.0
1	D	465	SER	2.0
1	B	296	HIS	2.0
1	B	11	ASN	2.0
1	B	190	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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,

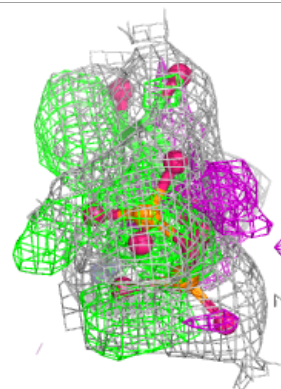
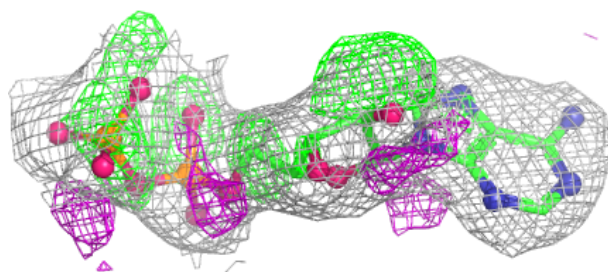
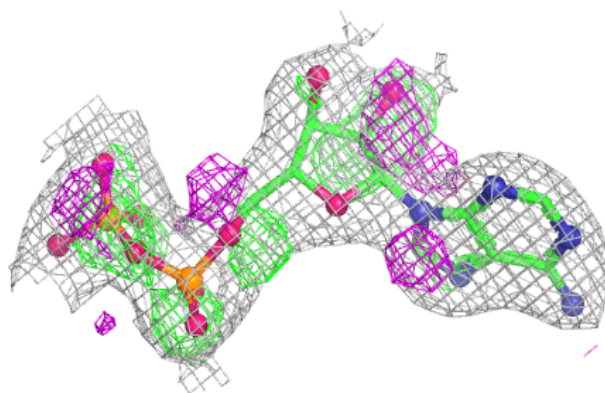
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	546	5/5	0.80	0.10	89,94,96,99	0
4	SO4	B	547	5/5	0.80	0.11	116,116,118,121	0
4	SO4	D	547	5/5	0.80	0.13	130,132,132,132	0
4	SO4	A	547	5/5	0.82	0.13	132,133,134,135	0
4	SO4	C	547	5/5	0.83	0.12	121,123,124,125	0
4	SO4	D	546	5/5	0.85	0.10	104,106,110,110	0
4	SO4	B	546	5/5	0.86	0.09	94,98,98,101	0
4	SO4	C	546	5/5	0.90	0.10	108,108,109,111	0
3	ADP	D	545	27/27	0.94	0.14	30,46,69,194	0
3	ADP	C	545	27/27	0.96	0.11	32,42,55,73	0
3	ADP	A	545	27/27	0.96	0.12	30,43,52,57	0
2	MG	D	544	1/1	0.97	0.05	39,39,39,39	0
3	ADP	B	545	27/27	0.97	0.12	35,52,71,74	0
2	MG	B	544	1/1	0.98	0.04	31,31,31,31	0
2	MG	C	544	1/1	0.99	0.04	27,27,27,27	0
2	MG	A	544	1/1	0.99	0.04	30,30,30,30	0

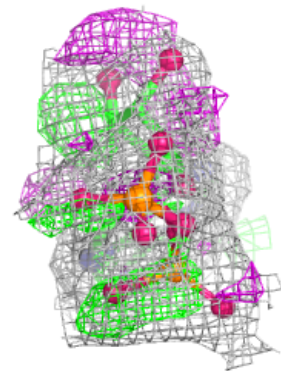
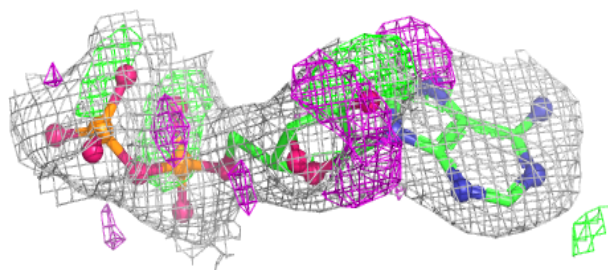
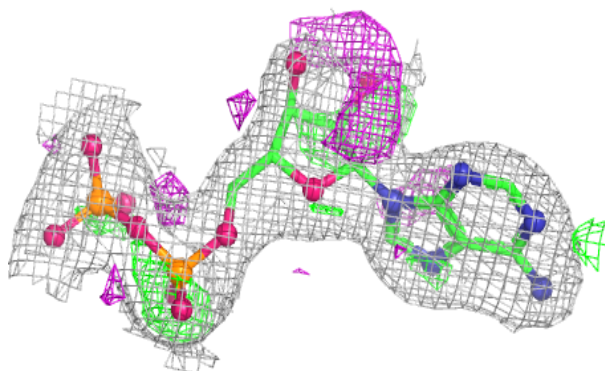
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 545:

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

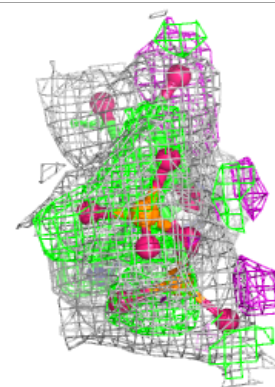
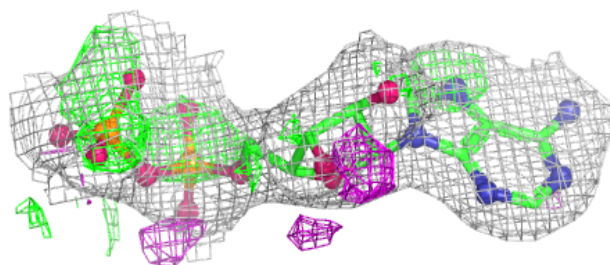
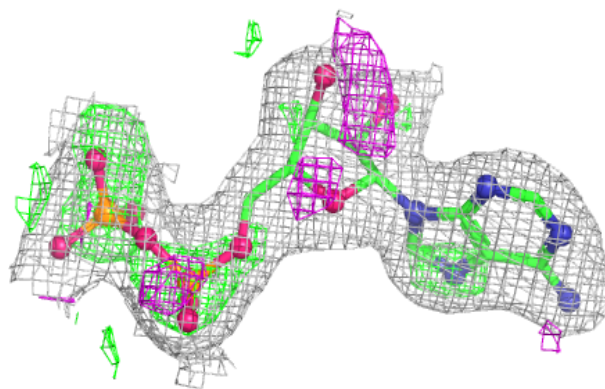
**Electron density around ADP C 545:**

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

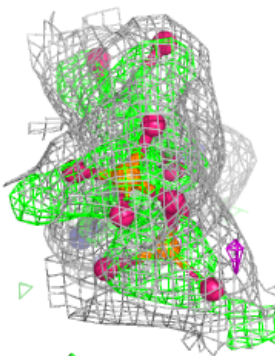
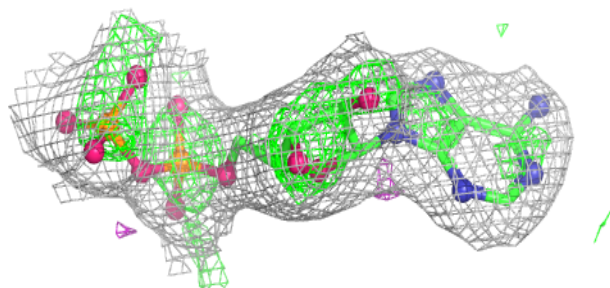
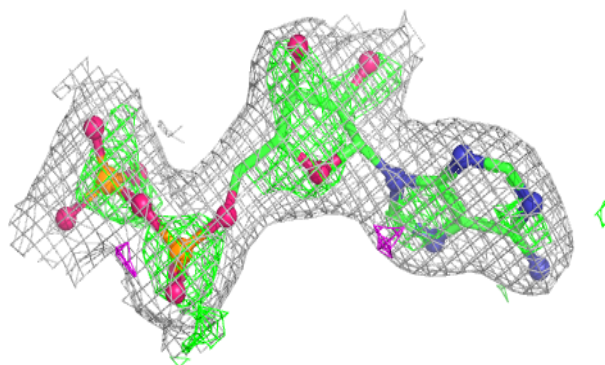


Electron density around ADP A 545:

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

**Electron density around ADP B 545:**

$2mF_o-DF_c$ (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.