



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:59 PM UTC

PDB ID : 3RUW / pdb_00003ruw
Title : Crystal structure of Cpn-rls in complex with ADP-AlF_x 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 : 2.70 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

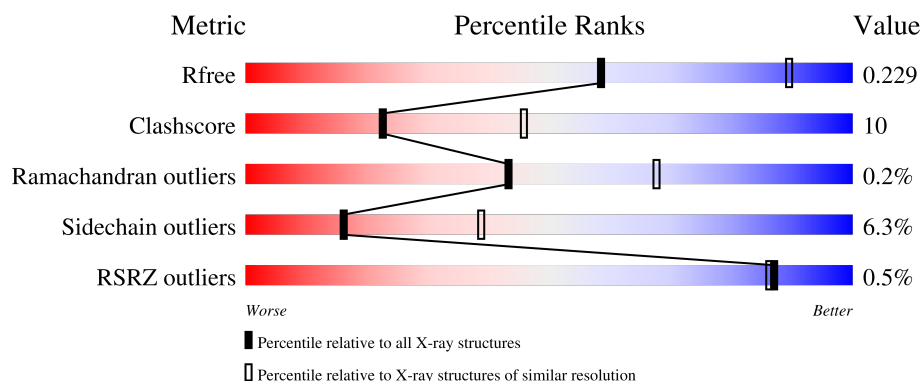
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	
1	B	543	
1	C	543	
1	D	543	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	548	-	-	X	-
5	SO4	C	548	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15720 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			

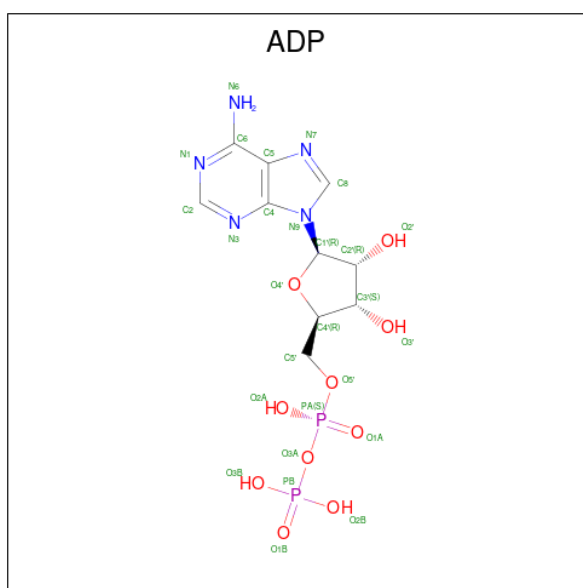
There are 16 discrepancies between the modelled and reference sequences:

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).

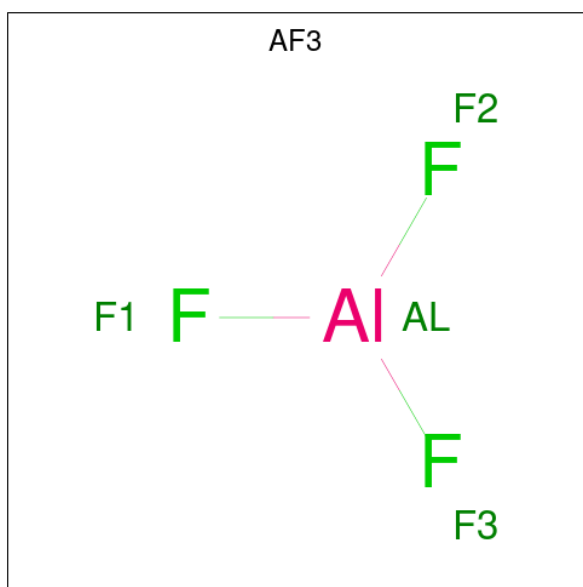
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

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



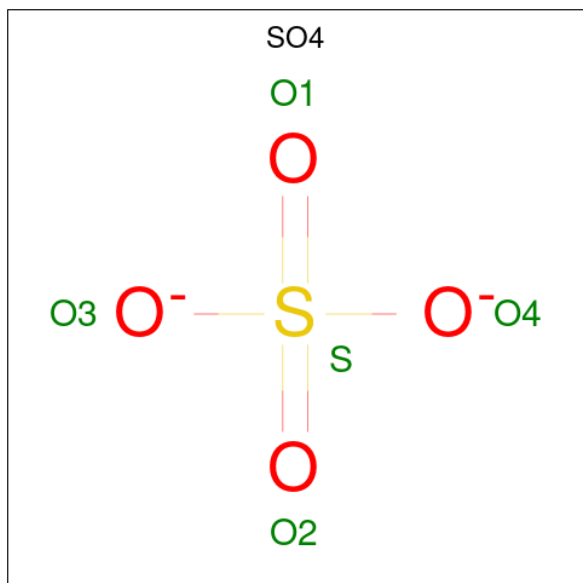
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0
3	C	1	Total C N O P 27 10 5 10 2	0	0
3	D	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			4	1	3		
4	B	1	Total	Al	F	0	0
			4	1	3		
4	C	1	Total	Al	F	0	0
			4	1	3		
4	D	1	Total	Al	F	0	0
			4	1	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

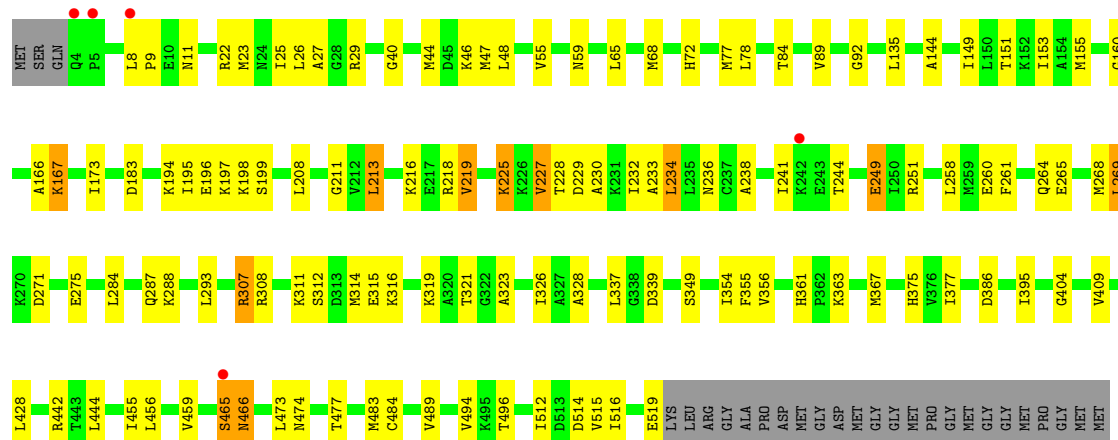


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

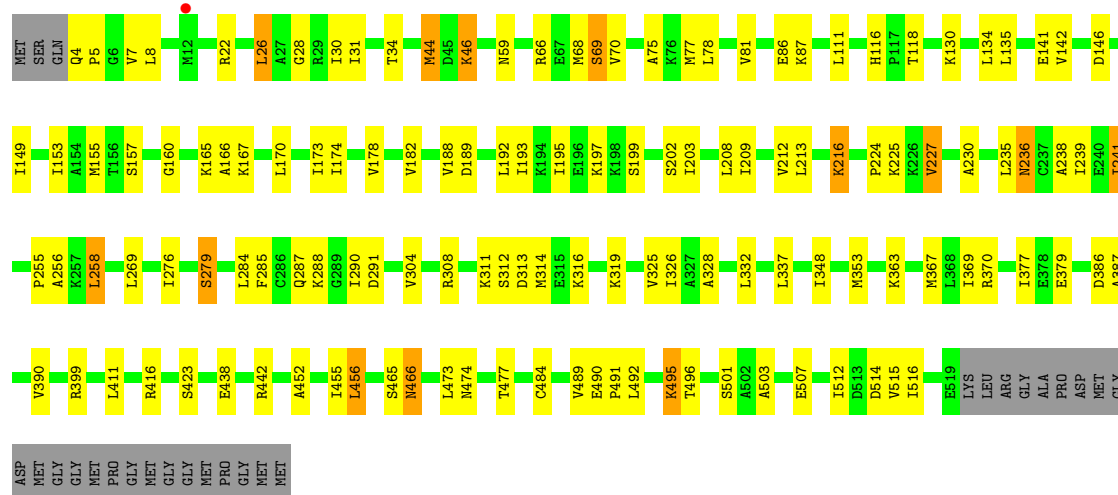
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	34	Total O 34 34	0	0
6	B	27	Total O 27 27	0	0
6	C	35	Total O 35 35	0	0
6	D	20	Total O 20 20	0	0

Chain C: 



• Molecule 1: Chaperonin

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	162.55Å 184.46Å 185.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 2.70 48.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.0 (48.97-2.70) 99.8 (48.97-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.172 , 0.227 0.179 , 0.229	Depositor DCC
R_{free} test set	3830 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15720	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: ADP, MG, AF3, SO4

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	0.47	0/3883	0.81	3/5228 (0.1%)
1	B	0.44	0/3883	0.80	2/5228 (0.0%)
1	C	0.45	0/3883	0.79	2/5228 (0.0%)
1	D	0.43	0/3883	0.77	0/5228
All	All	0.45	0/15532	0.79	7/20912 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	GLY	CA-C-N	6.69	126.95	119.32
1	C	40	GLY	C-N-CA	6.69	126.95	119.32
1	A	232	ILE	N-CA-C	5.46	115.81	108.17
1	B	40	GLY	CA-C-N	5.45	125.06	119.56
1	B	40	GLY	C-N-CA	5.45	125.06	119.56
1	A	357	GLU	N-CA-C	5.15	117.23	109.41
1	A	55	VAL	N-CA-C	5.11	116.07	108.46

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	75	0
1	B	3859	0	4001	91	0
1	C	3859	0	4001	95	0
1	D	3859	0	4001	104	0
2	A	1	0	0	0	0
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	3	0
3	B	27	0	12	1	0
3	C	27	0	12	4	0
3	D	27	0	12	1	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	10	0	0	1	0
5	B	10	0	0	6	0
5	C	10	0	0	4	0
5	D	10	0	0	1	0
6	A	34	0	0	5	0
6	B	27	0	0	3	0
6	C	35	0	0	8	0
6	D	20	0	0	6	0
All	All	15720	0	16052	332	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 10.

All (332) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LYS:CE	5:B:548:SO4:O4	1.64	1.46
1:B:225:LYS:HE3	5:B:548:SO4:O4	1.14	1.31
1:B:225:LYS:NZ	5:B:548:SO4:O4	1.89	1.06
1:A:375:HIS:HB3	1:B:508:MET:HE1	1.38	1.02
1:D:241:ILE:H	1:D:241:ILE:HD12	1.23	0.98
5:C:548:SO4:O2	1:D:319:LYS:HE2	1.63	0.97
1:D:160:GLY:O	6:D:556:HOH:O	1.83	0.96
1:C:386:ASP:OD1	6:C:554:HOH:O	1.83	0.93
1:B:382:ARG:NH1	6:B:572:HOH:O	2.05	0.88
3:C:545:ADP:H8	6:C:581:HOH:O	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASN:HD22	1:A:477:THR:HG23	1.45	0.82
1:B:160:GLY:O	6:B:552:HOH:O	1.98	0.81
1:C:59:ASN:OD1	6:C:551:HOH:O	1.98	0.81
1:A:122:LYS:HE3	1:A:426:GLU:OE1	1.79	0.81
1:C:48:LEU:HD23	1:D:516:ILE:HB	1.65	0.79
1:B:29:ARG:O	1:B:33:GLU:HG3	1.81	0.79
1:B:225:LYS:HE3	5:B:548:SO4:S	2.24	0.77
1:A:189:ASP:HB3	1:A:192:LEU:HD22	1.67	0.77
1:C:22:ARG:HD2	6:C:571:HOH:O	1.84	0.76
1:B:313:ASP:OD1	1:B:316:LYS:HE2	1.87	0.74
1:D:146:ASP:O	1:D:149:ILE:HG22	1.88	0.73
1:C:519:GLU:OE2	6:C:577:HOH:O	2.06	0.73
1:D:155:MET:HE1	1:D:166:ALA:HB1	1.69	0.73
1:C:234:LEU:HD22	1:C:323:ALA:HB3	1.70	0.72
1:B:259:MET:HE1	1:C:268:MET:HE1	1.71	0.72
1:D:238:ALA:HB2	1:D:288:LYS:HB2	1.71	0.72
1:B:293:LEU:HD13	1:C:328:ALA:HB2	1.72	0.71
1:B:189:ASP:HB3	1:B:192:LEU:HD22	1.72	0.71
1:A:160:GLY:O	6:A:552:HOH:O	2.09	0.70
1:A:293:LEU:HD13	1:B:328:ALA:HB2	1.73	0.69
1:A:251:ARG:NH1	1:B:249:GLU:HB2	2.07	0.69
1:C:271:ASP:O	1:C:275:GLU:HG3	1.93	0.69
1:C:225:LYS:HD2	5:C:548:SO4:O4	1.93	0.68
1:D:195:ILE:HG23	1:D:369:ILE:HD12	1.76	0.68
1:D:455:ILE:HD13	1:D:473:LEU:HD22	1.76	0.67
1:D:314:MET:HA	1:D:314:MET:HE2	1.76	0.67
1:A:271:ASP:O	1:A:275:GLU:HG3	1.95	0.67
1:D:203:ILE:HA	1:D:370:ARG:O	1.95	0.67
1:A:397:ASP:OD2	6:A:554:HOH:O	2.13	0.66
1:C:315:GLU:O	1:C:319:LYS:HG2	1.96	0.66
1:C:264:GLN:HA	1:C:264:GLN:HE21	1.61	0.66
1:C:349:SER:HB3	1:D:87:LYS:NZ	2.11	0.66
1:D:313:ASP:HA	1:D:316:LYS:HG2	1.77	0.66
1:A:234:LEU:HD22	1:A:323:ALA:HB3	1.78	0.66
1:D:225:LYS:HE3	5:D:548:SO4:O3	1.96	0.64
1:C:474:ASN:OD1	1:C:477:THR:HG23	1.98	0.63
1:A:375:HIS:CE1	1:B:77:MET:HE1	2.33	0.63
1:A:213:LEU:HD23	1:A:353:MET:HE1	1.81	0.63
1:B:30:ILE:O	1:B:34:THR:HG23	1.99	0.63
5:B:548:SO4:O2	1:C:319:LYS:NZ	2.23	0.62
1:B:313:ASP:HA	1:B:316:LYS:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:LEU:HD11	1:C:355:PHE:CD2	2.34	0.62
1:D:236:ASN:HB3	1:D:325:VAL:HG12	1.82	0.62
1:D:239:ILE:HD11	1:D:284:LEU:HD21	1.80	0.62
1:C:265:GLU:O	1:C:268:MET:HG2	2.00	0.61
1:C:287:GLN:O	1:C:308:ARG:HA	2.01	0.61
1:B:47:MET:HB2	1:C:512:ILE:HD13	1.83	0.61
1:C:153:ILE:HD13	1:C:489:VAL:HG23	1.82	0.61
1:C:483:MET:HE2	1:C:483:MET:HA	1.83	0.61
1:D:59:ASN:ND2	6:D:562:HOH:O	2.24	0.60
1:C:232:ILE:HD12	1:C:321:THR:HG21	1.82	0.60
1:A:116:HIS:HB3	1:A:119:ILE:HD12	1.83	0.60
1:D:474:ASN:OD1	1:D:477:THR:HG23	2.01	0.60
1:D:241:ILE:HD12	1:D:241:ILE:N	2.05	0.60
1:A:57:VAL:HG22	1:B:508:MET:HE2	1.83	0.59
1:A:519:GLU:OE2	6:A:576:HOH:O	2.17	0.59
1:B:66:ARG:NH2	1:B:86:GLU:OE2	2.34	0.59
1:D:241:ILE:H	1:D:241:ILE:CD1	2.01	0.59
1:C:173:ILE:HG23	1:C:208:LEU:HB2	1.82	0.59
1:D:287:GLN:HE22	1:D:311:LYS:HE3	1.67	0.59
1:A:215:ASP:HA	1:A:353:MET:HG2	1.84	0.59
1:A:313:ASP:OD1	1:A:316:LYS:HE2	2.03	0.59
1:A:194:LYS:HE3	1:A:316:LYS:HD3	1.85	0.58
1:D:386:ASP:OD1	6:D:565:HOH:O	2.17	0.58
1:A:315:GLU:O	1:A:319:LYS:HG2	2.03	0.58
1:B:89:VAL:HG11	1:B:494:VAL:HG22	1.85	0.57
1:D:285:PHE:HB3	1:D:314:MET:HE1	1.85	0.57
1:B:269:LEU:HD12	1:B:272:MET:HE3	1.86	0.57
1:C:44:MET:HE2	1:C:44:MET:HA	1.86	0.57
1:B:213:LEU:HD23	1:B:353:MET:CE	2.33	0.57
1:C:23:MET:HE3	1:C:72:HIS:HE2	1.69	0.57
1:B:31:ILE:HG13	1:B:75:ALA:HB1	1.86	0.57
3:D:545:ADP:H8	6:D:567:HOH:O	1.87	0.57
1:A:68:MET:HE2	1:B:516:ILE:CD1	2.35	0.57
1:B:173:ILE:HG23	1:B:208:LEU:HB2	1.87	0.57
1:C:23:MET:HE3	1:C:72:HIS:NE2	2.19	0.57
1:D:116:HIS:HD2	1:D:118:THR:OG1	1.87	0.57
1:D:213:LEU:HD23	1:D:353:MET:HE1	1.85	0.56
1:D:442:ARG:HG3	1:D:452:ALA:HB1	1.87	0.56
1:A:30:ILE:O	1:A:34:THR:HG23	2.06	0.56
1:D:153:ILE:HD13	1:D:489:VAL:HG23	1.88	0.56
1:A:48:LEU:HD13	1:A:67:GLU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLN:O	1:A:114:ASN:HB2	2.05	0.56
1:C:227:VAL:HG22	1:C:230:ALA:HB2	1.87	0.55
1:B:122:LYS:HD3	1:B:426:GLU:CD	2.32	0.55
1:A:409:VAL:HG11	1:A:459:VAL:HG12	1.88	0.54
1:B:9:PRO:HG2	1:B:12:MET:HE3	1.88	0.54
1:C:375:HIS:CE1	1:D:77:MET:HE1	2.42	0.54
1:D:238:ALA:HB2	1:D:288:LYS:CB	2.34	0.54
1:D:287:GLN:HE22	1:D:311:LYS:CE	2.20	0.54
1:D:141:GLU:HG2	1:D:399:ARG:NH1	2.22	0.54
1:B:46:LYS:HD2	1:C:514:ASP:HB3	1.89	0.54
1:D:279:SER:OG	1:D:332:LEU:HG	2.07	0.54
1:C:155:MET:HE1	1:C:166:ALA:O	2.07	0.54
1:C:455:ILE:HD12	1:C:473:LEU:HD13	1.90	0.54
1:D:4:GLN:N	1:D:5:PRO:HD3	2.23	0.54
1:D:209:ILE:HD12	1:D:213:LEU:HD11	1.89	0.54
1:B:69:SER:O	1:C:9:PRO:HG3	2.07	0.54
1:D:279:SER:HB3	1:D:337:LEU:HD11	1.89	0.54
1:B:270:LYS:HG2	1:B:297:TYR:CZ	2.42	0.54
1:B:360:LYS:C	1:B:362:PRO:HD3	2.33	0.54
1:C:233:ALA:O	1:C:284:LEU:HD12	2.08	0.54
1:B:259:MET:N	1:B:259:MET:HE2	2.23	0.53
1:C:409:VAL:HG11	1:C:459:VAL:HG12	1.89	0.53
1:A:89:VAL:HG22	1:A:493:ARG:HD2	1.90	0.53
1:C:236:ASN:O	1:C:288:LYS:HD3	2.08	0.53
1:D:495:LYS:NZ	6:D:551:HOH:O	2.42	0.53
1:D:189:ASP:HB3	1:D:192:LEU:CD1	2.39	0.53
1:C:199:SER:HA	1:C:377:ILE:HD11	1.89	0.52
1:A:189:ASP:HB3	1:A:192:LEU:CD2	2.37	0.52
1:D:130:LYS:O	1:D:134:LEU:HG	2.10	0.52
1:B:342:LEU:HD12	1:B:343:VAL:N	2.25	0.52
1:A:268:MET:O	1:A:272:MET:HG3	2.10	0.52
1:A:311:LYS:O	1:A:315:GLU:HG3	2.10	0.52
1:B:483:MET:HA	1:B:483:MET:HE2	1.92	0.52
1:D:28:GLY:HA2	1:D:78:LEU:HD22	1.92	0.52
1:D:313:ASP:OD1	1:D:316:LYS:HE2	2.10	0.51
1:B:234:LEU:HD12	1:B:285:PHE:HB2	1.92	0.51
1:D:4:GLN:N	1:D:5:PRO:CD	2.73	0.51
1:D:178:VAL:HA	1:D:193:ILE:HD11	1.91	0.51
1:D:189:ASP:HB3	1:D:192:LEU:HD12	1.92	0.51
1:C:249:GLU:HG2	1:C:251:ARG:HH12	1.74	0.51
1:C:241:ILE:HD11	1:C:269:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LEU:HD23	1:B:353:MET:HE3	1.91	0.51
1:C:238:ALA:HB2	1:C:288:LYS:HB3	1.93	0.50
1:A:211:GLY:HA3	1:A:356:VAL:O	2.10	0.50
1:C:234:LEU:HD22	1:C:323:ALA:CB	2.39	0.50
1:D:182:VAL:HG22	1:D:188:VAL:HG22	1.93	0.50
1:B:47:MET:HE2	1:C:515:VAL:HG22	1.92	0.50
1:D:22:ARG:O	1:D:26:LEU:HB2	2.11	0.50
1:D:66:ARG:NH2	1:D:86:GLU:OE1	2.44	0.50
1:C:213:LEU:HD11	1:C:355:PHE:CE2	2.46	0.50
1:D:348:ILE:HG21	1:D:353:MET:HE2	1.92	0.50
1:B:234:LEU:CD1	1:B:285:PHE:HB2	2.41	0.50
1:D:66:ARG:NH1	6:D:553:HOH:O	2.41	0.50
1:B:236:ASN:HA	1:B:287:GLN:HB3	1.94	0.50
1:C:89:VAL:HG11	1:C:494:VAL:HG22	1.94	0.49
1:C:219:VAL:HG23	1:C:307:ARG:HG2	1.92	0.49
1:C:92:GLY:HA2	3:C:545:ADP:PB	2.53	0.49
1:C:194:LYS:HE2	1:C:213:LEU:O	2.12	0.49
1:C:349:SER:HB3	1:D:87:LYS:HZ1	1.77	0.49
1:A:236:ASN:O	1:A:288:LYS:HE2	2.12	0.49
1:A:250:ILE:HD13	1:A:261:PHE:CD2	2.47	0.49
1:C:361:HIS:N	6:C:574:HOH:O	2.35	0.49
1:D:256:ALA:C	1:D:258:LEU:H	2.20	0.49
1:B:334:ALA:O	1:B:337:LEU:HB2	2.13	0.49
1:B:474:ASN:HD22	1:B:483:MET:HE1	1.76	0.49
1:D:492:LEU:O	1:D:496:THR:HG23	2.12	0.49
1:B:236:ASN:C	1:B:236:ASN:OD1	2.56	0.49
1:A:262:ILE:HD13	1:B:242:LYS:HB3	1.95	0.48
1:B:44:MET:HE2	1:B:44:MET:HA	1.94	0.48
1:A:161:LYS:O	1:A:165:LYS:NZ	2.43	0.48
1:C:27:ALA:HB2	1:C:72:HIS:CE1	2.49	0.48
1:D:30:ILE:O	1:D:34:THR:HG23	2.13	0.48
1:B:199:SER:HA	1:B:377:ILE:HD11	1.94	0.48
1:B:455:ILE:HD12	1:B:473:LEU:HD13	1.94	0.48
1:B:468:ASN:HB3	1:B:471:ALA:HB2	1.95	0.48
1:D:68:MET:O	1:D:69:SER:C	2.55	0.48
1:C:22:ARG:NH1	6:C:571:HOH:O	1.82	0.48
1:A:442:ARG:NH2	6:A:574:HOH:O	2.27	0.48
1:B:311:LYS:O	1:B:315:GLU:HG3	2.14	0.48
1:C:293:LEU:HD13	1:D:328:ALA:HB2	1.95	0.48
1:D:31:ILE:HG13	1:D:75:ALA:HB1	1.96	0.48
1:D:44:MET:HA	1:D:44:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:ILE:HG22	1:D:328:ALA:H	1.78	0.48
1:C:465:SER:O	1:C:466:ASN:C	2.57	0.47
1:D:313:ASP:CG	1:D:316:LYS:HE2	2.39	0.47
1:A:218:ARG:NH2	5:A:548:SO4:O3	2.38	0.47
1:A:342:LEU:HD21	1:A:344:GLU:HB2	1.97	0.47
1:C:25:ILE:O	1:C:29:ARG:HG3	2.14	0.47
1:C:197:LYS:O	1:C:198:LYS:HD2	2.13	0.47
1:C:287:GLN:N	1:C:314:MET:HE2	2.28	0.47
1:D:503:ALA:O	1:D:507:GLU:HG3	2.13	0.47
1:A:503:ALA:O	1:A:507:GLU:HG3	2.15	0.47
1:B:213:LEU:HD23	1:B:353:MET:HE1	1.97	0.47
1:C:264:GLN:HA	1:C:264:GLN:NE2	2.28	0.47
1:A:22:ARG:HG2	1:B:4:GLN:HE22	1.80	0.47
1:C:135:LEU:HD13	1:C:496:THR:HG22	1.97	0.47
1:C:195:ILE:HD13	1:C:367:MET:HB2	1.96	0.47
1:A:265:GLU:CD	1:B:244:THR:HG22	2.39	0.47
1:D:197:LYS:HB3	1:D:377:ILE:HG21	1.96	0.47
1:C:319:LYS:O	1:C:363:LYS:HB2	2.14	0.47
1:A:92:GLY:HA2	3:A:545:ADP:PB	2.55	0.46
1:B:216:LYS:O	1:B:354:ILE:HG13	2.16	0.46
1:A:64:ILE:CG2	1:A:68:MET:HE3	2.45	0.46
1:B:259:MET:HE1	1:C:268:MET:CE	2.43	0.46
1:B:431:ARG:O	1:B:434:ALA:HB3	2.16	0.46
1:B:448:ALA:HB2	1:B:475:VAL:HG12	1.97	0.46
1:A:474:ASN:ND2	1:A:477:THR:HG23	2.22	0.46
1:C:404:GLY:HA2	3:C:545:ADP:N3	2.31	0.46
1:D:173:ILE:HG23	1:D:208:LEU:HB2	1.96	0.46
1:B:442:ARG:HB2	1:B:456:LEU:HD11	1.97	0.46
1:C:287:GLN:CA	1:C:314:MET:HE2	2.46	0.46
1:D:379:GLU:OE2	1:D:379:GLU:HA	2.16	0.46
1:D:442:ARG:HG3	1:D:452:ALA:CB	2.46	0.46
1:D:495:LYS:N	1:D:495:LYS:HD2	2.31	0.46
1:A:8:LEU:HD13	1:A:12:MET:HE1	1.98	0.46
1:A:64:ILE:HG22	1:A:68:MET:HE3	1.98	0.46
1:B:153:ILE:HD13	1:B:489:VAL:HG23	1.97	0.46
1:C:47:MET:HE2	1:D:515:VAL:HG22	1.96	0.46
1:C:65:LEU:HD23	1:C:68:MET:CE	2.46	0.46
1:A:455:ILE:HD12	1:A:473:LEU:HD13	1.97	0.46
1:C:218:ARG:CZ	1:C:225:LYS:HG3	2.46	0.46
1:D:276:ILE:O	1:D:279:SER:HB2	2.16	0.46
1:A:46:LYS:HD2	1:B:514:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ASP:OD1	1:C:183:ASP:C	2.60	0.45
1:D:155:MET:CE	1:D:166:ALA:HB1	2.42	0.45
1:D:216:LYS:HE3	1:D:308:ARG:O	2.15	0.45
1:A:110:LEU:HD21	1:A:429:ALA:HA	1.99	0.45
1:B:9:PRO:HG2	1:B:12:MET:CE	2.45	0.45
1:B:78:LEU:O	1:B:81:VAL:HB	2.16	0.45
1:D:239:ILE:CD1	1:D:284:LEU:HD21	2.46	0.45
1:A:342:LEU:CD2	1:A:344:GLU:HB2	2.46	0.45
1:D:416:ARG:HH22	1:D:438:GLU:CD	2.24	0.45
1:B:308:ARG:NH1	5:B:547:SO4:O1	2.50	0.45
1:D:239:ILE:HG22	1:D:239:ILE:O	2.17	0.45
1:A:15:TYR:O	1:A:20:ALA:HB2	2.16	0.45
1:D:174:ILE:HD13	1:D:387:ALA:HB3	1.98	0.45
1:C:228:THR:O	1:C:229:ASP:C	2.59	0.45
1:D:442:ARG:HH11	1:D:442:ARG:HG2	1.82	0.45
1:C:264:GLN:O	1:C:268:MET:HE3	2.17	0.44
1:C:349:SER:HB3	1:D:87:LYS:HZ3	1.82	0.44
1:C:455:ILE:HD13	1:C:455:ILE:HA	1.82	0.44
1:B:130:LYS:O	1:B:134:LEU:HG	2.17	0.44
1:B:375:HIS:CE1	1:C:77:MET:HE1	2.52	0.44
1:C:27:ALA:HA	1:D:7:VAL:HG21	1.98	0.44
1:C:199:SER:O	1:C:349:SER:OG	2.36	0.44
1:C:269:LEU:HD12	1:C:269:LEU:HA	1.89	0.44
1:D:465:SER:O	1:D:466:ASN:C	2.61	0.44
1:D:165:LYS:HE2	1:D:379:GLU:HG3	1.98	0.44
1:D:195:ILE:HD13	1:D:367:MET:HB2	2.00	0.44
1:A:27:ALA:HA	1:B:7:VAL:HG21	1.99	0.44
1:A:57:VAL:CG2	1:B:508:MET:HE2	2.47	0.44
1:B:293:LEU:HG	1:B:297:TYR:CE2	2.52	0.44
1:D:199:SER:HA	1:D:377:ILE:HD11	1.98	0.44
1:B:194:LYS:HG3	1:B:316:LYS:HD2	1.99	0.44
1:B:255:PRO:HA	1:C:261:PHE:CE2	2.53	0.44
1:D:81:VAL:HG13	1:D:501:SER:HB3	2.00	0.44
1:A:372:THR:O	1:B:84:THR:HG21	2.18	0.43
1:C:167:LYS:HD2	1:C:167:LYS:N	2.32	0.43
1:D:287:GLN:NE2	1:D:311:LYS:HE3	2.33	0.43
1:A:411:LEU:HA	1:A:411:LEU:HD23	1.73	0.43
1:A:466:ASN:N	1:A:466:ASN:HD22	2.16	0.43
1:B:189:ASP:HB3	1:B:192:LEU:CD2	2.44	0.43
1:C:160:GLY:O	6:C:551:HOH:O	2.21	0.43
1:C:216:LYS:O	1:C:354:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:GLN:HB2	1:C:314:MET:HE2	2.00	0.43
3:A:545:ADP:H8	6:A:577:HOH:O	2.01	0.43
1:D:135:LEU:HD21	1:D:411:LEU:HD22	2.01	0.43
1:D:235:LEU:HD23	1:D:326:ILE:HB	2.00	0.43
1:B:307:ARG:HD2	1:B:308:ARG:CZ	2.49	0.43
1:B:360:LYS:O	1:B:362:PRO:HD3	2.19	0.43
1:C:442:ARG:HD3	1:C:456:LEU:HD22	2.00	0.43
1:A:219:VAL:HG21	1:A:295:GLN:CD	2.43	0.43
1:D:68:MET:HG3	1:D:70:VAL:HG23	2.00	0.43
1:C:151:THR:O	1:C:155:MET:HG2	2.19	0.43
1:C:307:ARG:HG3	5:C:547:SO4:O3	2.19	0.43
1:B:160:GLY:HA3	6:B:574:HOH:O	2.18	0.42
1:B:236:ASN:HB3	1:B:325:VAL:CG1	2.49	0.42
1:A:450:LEU:HD12	1:A:473:LEU:HD21	2.01	0.42
1:B:194:LYS:HE3	1:B:316:LYS:CB	2.49	0.42
1:C:232:ILE:O	1:C:337:LEU:HA	2.19	0.42
1:B:270:LYS:HE3	1:B:297:TYR:CE1	2.54	0.42
1:A:14:ARG:HG3	1:A:516:ILE:HG12	2.01	0.42
1:A:275:GLU:OE2	1:A:330:ALA:HA	2.19	0.42
1:B:149:ILE:HD12	1:B:152:LYS:HD2	2.01	0.42
1:B:194:LYS:HE3	1:B:316:LYS:HB2	2.01	0.42
1:D:238:ALA:CB	1:D:288:LYS:HB2	2.45	0.42
1:D:290:ILE:O	1:D:291:ASP:C	2.61	0.42
1:D:135:LEU:HD13	1:D:496:THR:HG22	2.01	0.42
1:D:157:SER:HB2	1:D:390:VAL:HG21	2.02	0.42
1:C:46:LYS:HD2	1:D:514:ASP:HB3	2.01	0.42
1:D:390:VAL:HG12	1:D:491:PRO:HG2	2.00	0.42
1:A:232:ILE:HD12	1:A:321:THR:HG21	2.01	0.42
1:C:27:ALA:CB	1:C:72:HIS:CE1	3.03	0.42
1:C:311:LYS:O	1:C:315:GLU:HG3	2.20	0.42
1:A:379:GLU:HA	1:A:379:GLU:OE1	2.19	0.42
1:A:456:LEU:O	1:A:460:ARG:HB2	2.18	0.42
1:B:477:THR:HG21	1:B:481:GLU:OE1	2.20	0.42
1:C:47:MET:HB2	1:D:512:ILE:HD13	2.01	0.42
1:D:141:GLU:HG2	1:D:399:ARG:HH11	1.84	0.42
1:A:18:ARG:HH22	1:A:108:GLU:HG3	1.85	0.42
1:B:284:LEU:HD12	1:B:285:PHE:N	2.35	0.42
1:B:255:PRO:HG2	1:C:260:GLU:HG2	2.02	0.41
1:C:47:MET:HE2	1:D:515:VAL:CG2	2.50	0.41
1:D:227:VAL:CG2	1:D:230:ALA:HB2	2.50	0.41
1:D:255:PRO:O	1:D:258:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HG13	1:A:75:ALA:HB1	2.01	0.41
1:B:348:ILE:O	1:B:349:SER:HB2	2.20	0.41
1:D:455:ILE:HD13	1:D:473:LEU:CD2	2.48	0.41
1:B:68:MET:HE1	1:C:516:ILE:HD13	2.01	0.41
1:C:211:GLY:HA3	1:C:356:VAL:O	2.21	0.41
5:C:548:SO4:S	1:D:319:LYS:HE2	2.58	0.41
1:D:224:PRO:HG2	1:D:304:VAL:HG23	2.02	0.41
1:A:50:ASP:OD2	1:A:54:ASP:HB2	2.21	0.41
1:C:144:ALA:HB1	1:C:395:ILE:HG23	2.02	0.41
1:D:34:THR:O	1:D:46:LYS:HE2	2.21	0.41
1:B:265:GLU:O	1:B:269:LEU:HD22	2.20	0.41
1:B:518:ALA:O	1:B:519:GLU:C	2.64	0.41
1:A:123:GLY:HA3	1:A:429:ALA:HB3	2.02	0.41
1:A:249:GLU:HG2	1:A:251:ARG:HH12	1.85	0.41
1:B:404:GLY:HA2	3:B:545:ADP:N3	2.36	0.41
1:A:404:GLY:HA2	3:A:545:ADP:N3	2.36	0.41
1:C:92:GLY:HA2	3:C:545:ADP:O3B	2.21	0.41
1:A:18:ARG:HH22	1:A:108:GLU:CG	2.34	0.41
1:A:27:ALA:HB2	1:A:72:HIS:CE1	2.56	0.41
1:A:70:VAL:HG21	1:A:79:ILE:HD11	2.03	0.41
1:B:269:LEU:CD1	1:B:272:MET:HE3	2.51	0.41
1:D:452:ALA:O	1:D:456:LEU:HB2	2.20	0.41
1:A:167:LYS:HB3	1:A:167:LYS:HE3	1.97	0.40
1:A:199:SER:HA	1:A:377:ILE:HD11	2.03	0.40
1:C:194:LYS:HE3	1:C:196:GLU:OE1	2.22	0.40
1:D:167:LYS:HA	1:D:167:LYS:HD2	1.86	0.40
1:A:78:LEU:O	1:A:81:VAL:HB	2.21	0.40
1:C:444:LEU:HA	1:C:444:LEU:HD23	1.81	0.40
1:D:363:LYS:HD3	1:D:363:LYS:HA	1.83	0.40
1:A:159:THR:O	1:A:162:GLY:N	2.52	0.40
1:B:136:LYS:O	1:B:399:ARG:NH2	2.54	0.40
1:B:211:GLY:HA3	1:B:356:VAL:O	2.22	0.40
1:A:164:GLU:OE2	1:B:511:ARG:HD2	2.22	0.40
1:D:195:ILE:CG2	1:D:369:ILE:HD12	2.48	0.40
1:D:411:LEU:HD12	1:D:411:LEU:HA	1.89	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	514/543 (95%)	495 (96%)	19 (4%)	0	100	100
1	B	514/543 (95%)	494 (96%)	20 (4%)	0	100	100
1	C	514/543 (95%)	499 (97%)	13 (2%)	2 (0%)	30	54
1	D	514/543 (95%)	492 (96%)	20 (4%)	2 (0%)	30	54
All	All	2056/2172 (95%)	1980 (96%)	72 (4%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	465	SER
1	D	466	ASN
1	C	466	ASN
1	D	69	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%)	386 (94%)	26 (6%)	16	39
1	B	412/430 (96%)	380 (92%)	32 (8%)	11	29
1	C	412/430 (96%)	388 (94%)	24 (6%)	18	42
1	D	412/430 (96%)	390 (95%)	22 (5%)	20	46
All	All	1648/1720 (96%)	1544 (94%)	104 (6%)	16	39

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	12	MET
1	A	13	LYS
1	A	31	ILE
1	A	42	LYS
1	A	55	VAL
1	A	57	VAL
1	A	78	LEU
1	A	110	LEU
1	A	120	VAL
1	A	149	ILE
1	A	167	LYS
1	A	192	LEU
1	A	206	THR
1	A	234	LEU
1	A	269	LEU
1	A	307	ARG
1	A	312	SER
1	A	342	LEU
1	A	352	SER
1	A	428	LEU
1	A	456	LEU
1	A	466	ASN
1	A	484	CYS
1	A	490	GLU
1	A	510	LEU
1	B	8	LEU
1	B	12	MET
1	B	57	VAL
1	B	78	LEU
1	B	121	VAL
1	B	122	LYS
1	B	137	THR
1	B	142	VAL
1	B	149	ILE
1	B	167	LYS
1	B	170	LEU
1	B	190	LYS
1	B	192	LEU
1	B	228	THR
1	B	234	LEU
1	B	244	THR

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Mol	Chain	Res	Type
1	B	258	LEU
1	B	259	MET
1	B	269	LEU
1	B	284	LEU
1	B	307	ARG
1	B	310	LYS
1	B	337	LEU
1	B	411	LEU
1	B	423	SER
1	B	437	LEU
1	B	444	LEU
1	B	450	LEU
1	B	475	VAL
1	B	480	VAL
1	B	483	MET
1	B	484	CYS
1	C	8	LEU
1	C	11	ASN
1	C	26	LEU
1	C	55	VAL
1	C	78	LEU
1	C	84	THR
1	C	149	ILE
1	C	167	LYS
1	C	213	LEU
1	C	219	VAL
1	C	225	LYS
1	C	227	VAL
1	C	234	LEU
1	C	244	THR
1	C	249	GLU
1	C	258	LEU
1	C	269	LEU
1	C	307	ARG
1	C	312	SER
1	C	316	LYS
1	C	326	ILE
1	C	339	ASP
1	C	428	LEU
1	C	484	CYS
1	D	8	LEU
1	D	26	LEU

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Mol	Chain	Res	Type
1	D	44	MET
1	D	46	LYS
1	D	111	LEU
1	D	142	VAL
1	D	170	LEU
1	D	202	SER
1	D	212	VAL
1	D	216	LYS
1	D	227	VAL
1	D	236	ASN
1	D	241	ILE
1	D	258	LEU
1	D	269	LEU
1	D	279	SER
1	D	312	SER
1	D	423	SER
1	D	456	LEU
1	D	484	CYS
1	D	490	GLU
1	D	495	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	11	ASN
1	A	264	GLN
1	A	427	GLN
1	A	466	ASN
1	A	474	ASN
1	A	500	GLN
1	B	4	GLN
1	B	264	GLN
1	B	287	GLN
1	B	296	HIS
1	B	427	GLN
1	B	474	ASN
1	B	500	GLN
1	C	4	GLN
1	C	11	ASN
1	C	125	GLN
1	C	236	ASN

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Mol	Chain	Res	Type
1	C	264	GLN
1	C	287	GLN
1	C	296	HIS
1	C	361	HIS
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	324	ASN
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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	D	545	2	28,29,29	1.35	4 (14%)	43,45,45	1.81	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	D	548	-	4,4,4	0.29	0	6,6,6	0.36	0
4	AF3	C	546	-	0,3,3	-	-	-		
5	SO4	C	547	-	4,4,4	0.28	0	6,6,6	0.15	0
5	SO4	A	547	-	4,4,4	0.21	0	6,6,6	0.16	0
5	SO4	B	547	-	4,4,4	0.23	0	6,6,6	0.19	0
3	ADP	C	545	2	28,29,29	1.52	5 (17%)	43,45,45	1.87	10 (23%)
4	AF3	A	546	-	0,3,3	-	-	-		
3	ADP	B	545	2	28,29,29	1.49	5 (17%)	43,45,45	1.81	9 (20%)
4	AF3	B	546	-	0,3,3	-	-	-		
4	AF3	D	546	-	0,3,3	-	-	-		
5	SO4	B	548	-	4,4,4	0.32	0	6,6,6	0.41	0
5	SO4	D	547	-	4,4,4	0.26	0	6,6,6	0.15	0
5	SO4	C	548	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	A	548	-	4,4,4	0.34	0	6,6,6	0.29	0
3	ADP	A	545	2	28,29,29	1.45	6 (21%)	43,45,45	1.87	11 (25%)

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	C	545	2	-	2/16/32/32	0/3/3/3
3	ADP	B	545	2	-	2/16/32/32	0/3/3/3
3	ADP	D	545	2	-	5/16/32/32	0/3/3/3
3	ADP	A	545	2	-	2/16/32/32	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	4.64	1.47	1.39
3	B	545	ADP	C5-C4	4.52	1.47	1.39
3	D	545	ADP	C5-C4	4.37	1.46	1.39
3	A	545	ADP	C5-C4	4.29	1.46	1.39
3	C	545	ADP	PA-O3A	3.25	1.63	1.59
3	B	545	ADP	PA-O3A	2.92	1.62	1.59
3	A	545	ADP	PA-O3A	2.89	1.62	1.59
3	B	545	ADP	C8-N7	2.75	1.37	1.31
3	B	545	ADP	C5-C6	2.70	1.48	1.41
3	C	545	ADP	C8-N7	2.66	1.36	1.31
3	C	545	ADP	C5-C6	2.64	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	545	ADP	C5-N7	-2.51	1.34	1.39
3	A	545	ADP	C5-C6	2.47	1.47	1.41
3	A	545	ADP	C5-N7	-2.46	1.34	1.39
3	D	545	ADP	C5-C6	2.43	1.47	1.41
3	C	545	ADP	C5-N7	-2.25	1.35	1.39
3	D	545	ADP	C8-N7	2.20	1.35	1.31
3	D	545	ADP	C5-N7	-2.20	1.35	1.39
3	A	545	ADP	C4-N9	-2.19	1.33	1.37
3	A	545	ADP	C8-N7	2.17	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	-6.16	118.23	126.72
3	D	545	ADP	C5-C4-N3	-5.60	119.01	126.72
3	C	545	ADP	C5-C4-N3	-5.58	119.03	126.72
3	A	545	ADP	C5-C4-N3	-5.41	119.27	126.72
3	D	545	ADP	N3-C4-N9	4.98	135.64	127.17
3	B	545	ADP	N3-C4-N9	4.46	134.75	127.17
3	A	545	ADP	N3-C4-N9	4.40	134.64	127.17
3	C	545	ADP	N3-C4-N9	4.34	134.55	127.17
3	B	545	ADP	C2-N3-C4	3.87	121.29	111.83
3	B	545	ADP	C4-C5-N7	-3.67	106.38	110.58
3	C	545	ADP	C2-N3-C4	3.64	120.73	111.83
3	A	545	ADP	C2-N3-C4	3.62	120.67	111.83
3	C	545	ADP	O4'-C1'-N9	3.60	115.00	108.09
3	D	545	ADP	C2-N3-C4	3.58	120.57	111.83
3	A	545	ADP	N3-C2-N1	-3.53	123.24	128.58
3	C	545	ADP	C4-C5-N7	-3.42	106.68	110.58
3	A	545	ADP	O4'-C1'-N9	3.41	114.63	108.09
3	D	545	ADP	C4-N9-C8	3.38	109.29	105.74
3	A	545	ADP	C4-C5-N7	-3.28	106.84	110.58
3	C	545	ADP	N3-C2-N1	-3.20	123.74	128.58
3	D	545	ADP	N3-C2-N1	-3.13	123.85	128.58
3	B	545	ADP	N3-C2-N1	-3.13	123.85	128.58
3	A	545	ADP	C4-N9-C8	3.07	108.97	105.74
3	C	545	ADP	C4-N9-C8	2.78	108.66	105.74
3	D	545	ADP	C4-C5-N7	-2.67	107.53	110.58
3	B	545	ADP	C5-N7-C8	2.60	107.53	103.45
3	C	545	ADP	C5-N7-C8	2.51	107.40	103.45
3	A	545	ADP	C5-N7-C8	2.51	107.39	103.45
3	C	545	ADP	C6-C5-N7	2.31	136.54	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	545	ADP	C5-N7-C8	2.30	107.07	103.45
3	D	545	ADP	N6-C6-N1	2.27	123.42	118.38
3	A	545	ADP	N9-C8-N7	-2.25	110.74	113.94
3	B	545	ADP	O4'-C1'-N9	2.24	112.39	108.09
3	D	545	ADP	N9-C8-N7	-2.23	110.77	113.94
3	A	545	ADP	C2-N1-C6	2.19	122.33	118.73
3	C	545	ADP	N9-C8-N7	-2.17	110.85	113.94
3	B	545	ADP	C6-C5-N7	2.15	136.24	132.09
3	A	545	ADP	C6-C5-N7	2.14	136.22	132.09
3	B	545	ADP	C4-N9-C8	2.05	107.89	105.74

There are no chirality outliers.

All (11) torsion outliers are listed below:

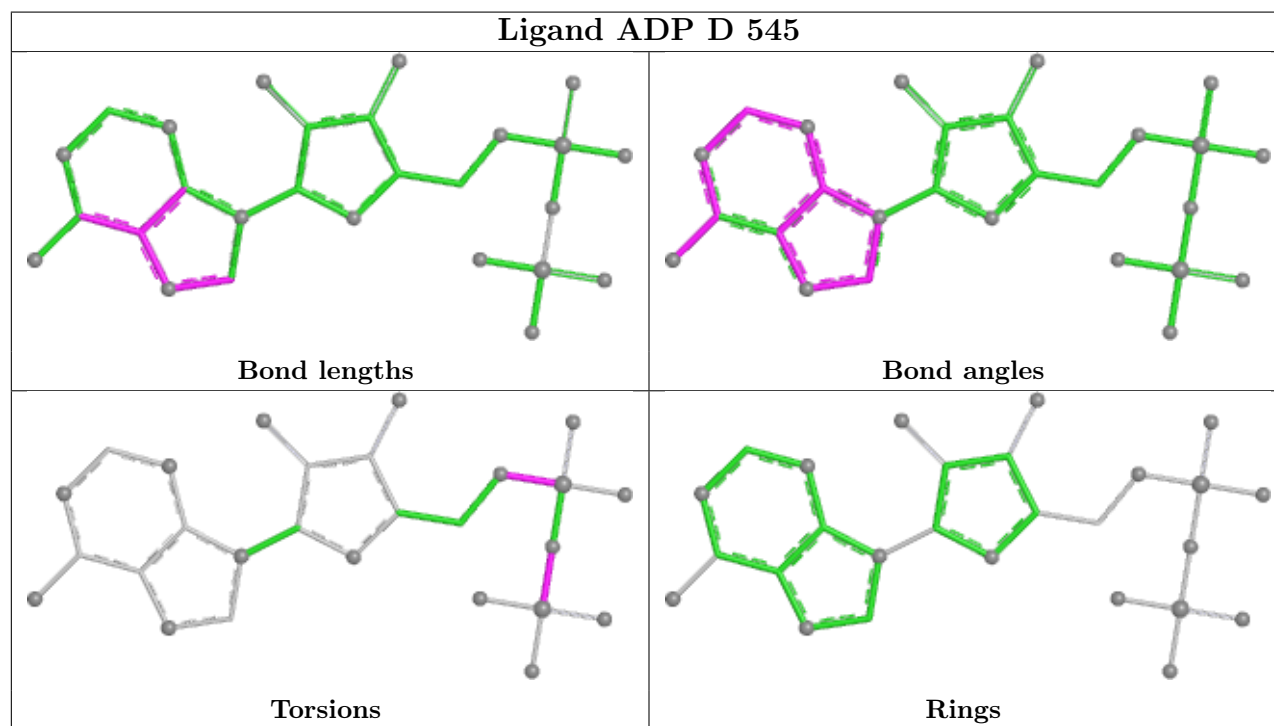
Mol	Chain	Res	Type	Atoms
3	D	545	ADP	C5'-O5'-PA-O2A
3	C	545	ADP	PB-O3A-PA-O1A
3	D	545	ADP	PA-O3A-PB-O1B
3	B	545	ADP	PB-O3A-PA-O2A
3	D	545	ADP	C5'-O5'-PA-O3A
3	A	545	ADP	PB-O3A-PA-O1A
3	A	545	ADP	PB-O3A-PA-O2A
3	C	545	ADP	PB-O3A-PA-O2A
3	D	545	ADP	PA-O3A-PB-O2B
3	D	545	ADP	PA-O3A-PB-O3B
3	B	545	ADP	PB-O3A-PA-O1A

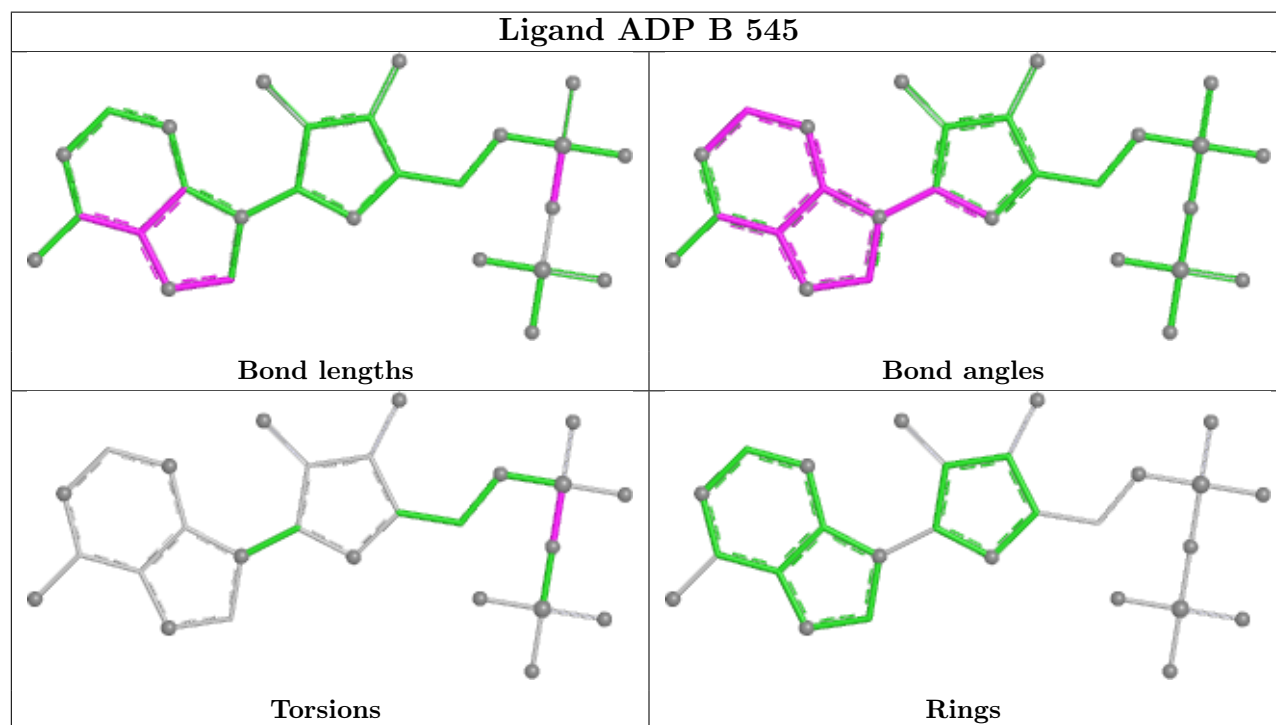
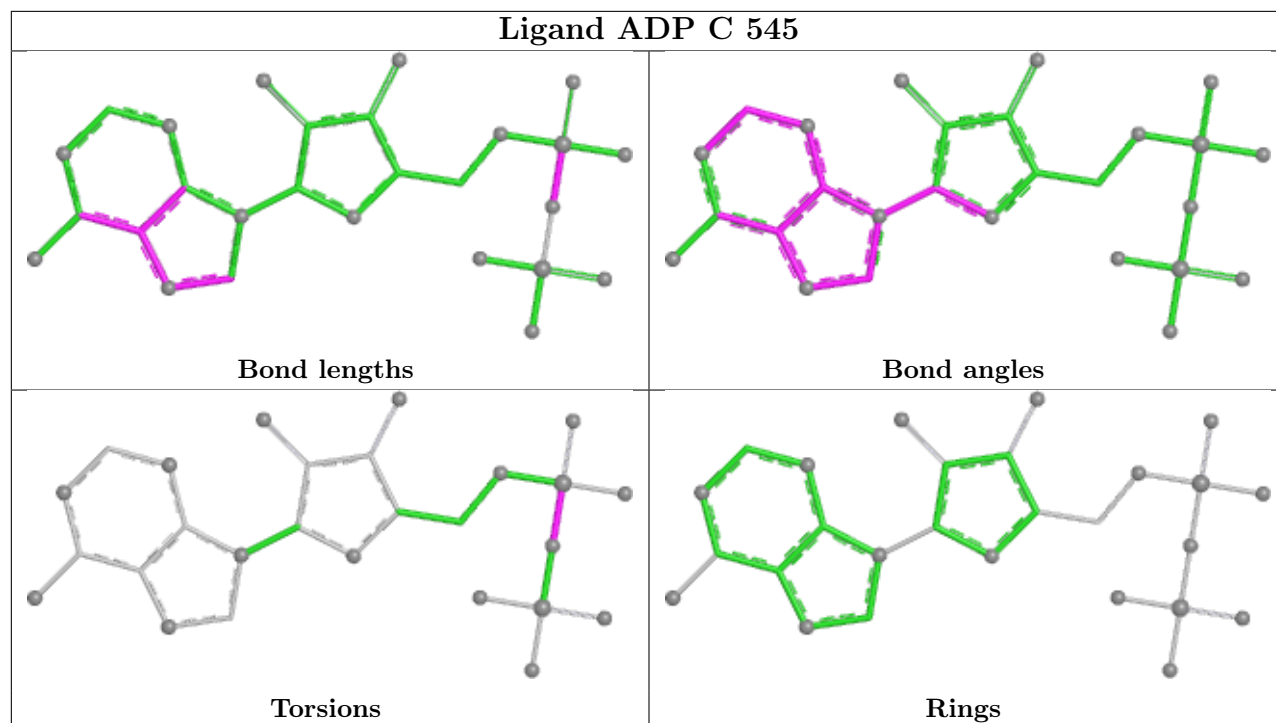
There are no ring outliers.

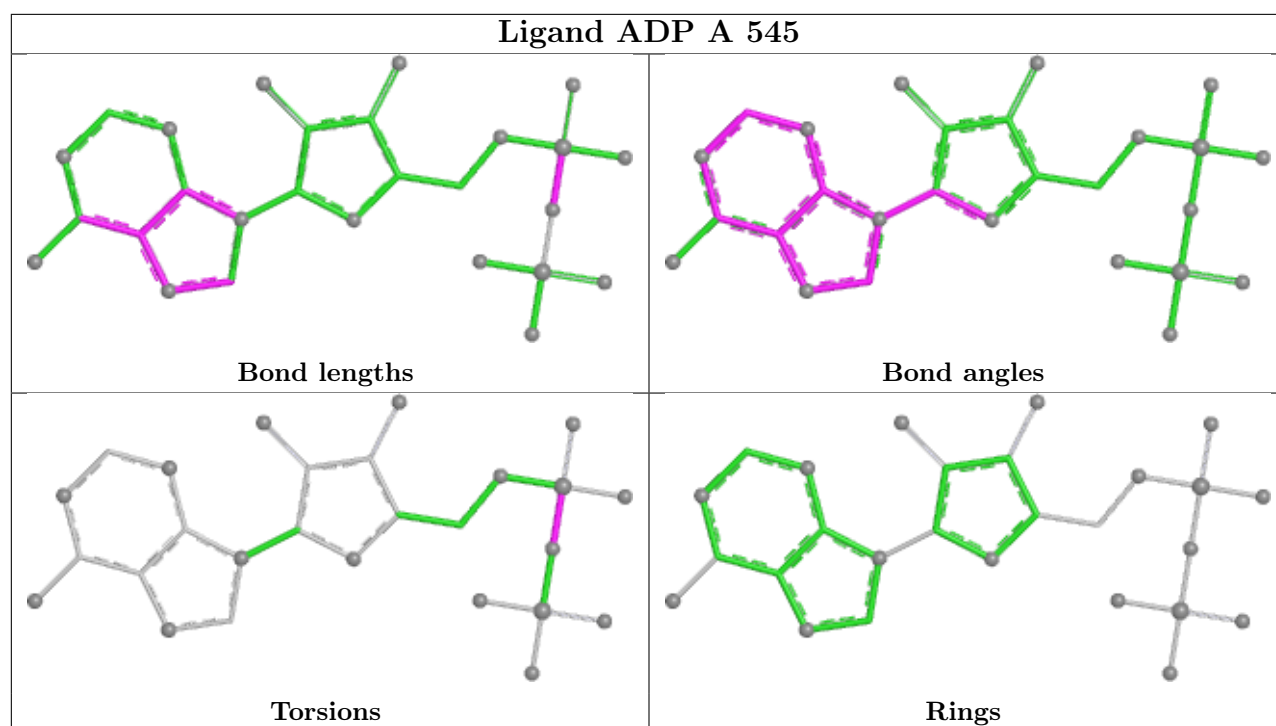
10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	545	ADP	1	0
5	D	548	SO4	1	0
5	C	547	SO4	1	0
5	B	547	SO4	1	0
3	C	545	ADP	4	0
3	B	545	ADP	1	0
5	B	548	SO4	5	0
5	C	548	SO4	3	0
5	A	548	SO4	1	0
3	A	545	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	516/543 (95%)	-0.41	1 (0%) 91 90	29, 58, 96, 135	0
1	B	516/543 (95%)	-0.37	4 (0%) 82 81	28, 59, 99, 142	0
1	C	516/543 (95%)	-0.37	5 (0%) 79 78	29, 60, 101, 144	0
1	D	516/543 (95%)	-0.33	1 (0%) 91 90	33, 64, 100, 141	0
All	All	2064/2172 (95%)	-0.37	11 (0%) 87 86	28, 60, 99, 144	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	PRO	3.6
1	B	8	LEU	3.0
1	A	5	PRO	2.6
1	B	12	MET	2.5
1	C	242	LYS	2.3
1	B	4	GLN	2.2
1	B	5	PRO	2.2
1	C	4	GLN	2.1
1	C	465	SER	2.1
1	D	12	MET	2.1
1	C	8	LEU	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

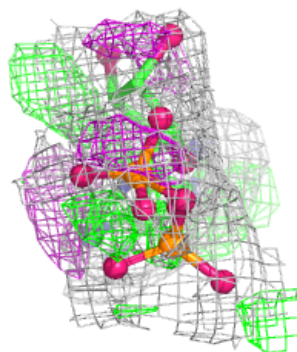
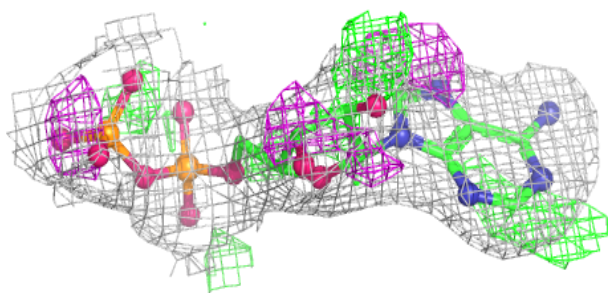
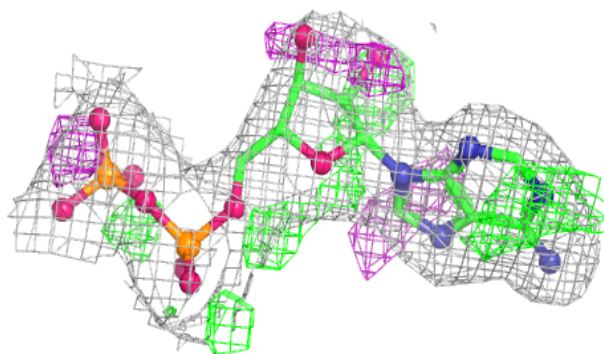
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	C	547	5/5	0.69	0.13	113,116,119,119	0
5	SO4	A	548	5/5	0.71	0.11	139,140,141,141	0
5	SO4	A	547	5/5	0.72	0.12	118,118,121,122	0
5	SO4	D	548	5/5	0.78	0.09	145,150,150,150	0
5	SO4	B	548	5/5	0.81	0.09	137,140,144,144	0
5	SO4	C	548	5/5	0.82	0.10	114,123,127,128	0
5	SO4	B	547	5/5	0.82	0.09	110,117,119,121	0
5	SO4	D	547	5/5	0.83	0.08	104,105,107,114	0
4	AF3	A	546	4/4	0.92	0.11	44,45,55,58	0
4	AF3	B	546	4/4	0.93	0.13	42,46,63,71	0
3	ADP	C	545	27/27	0.95	0.10	26,44,60,60	0
3	ADP	D	545	27/27	0.95	0.10	32,55,80,162	0
2	MG	D	544	1/1	0.95	0.07	56,56,56,56	0
4	AF3	D	546	4/4	0.96	0.06	40,50,51,57	0
3	ADP	A	545	27/27	0.97	0.07	26,45,53,56	0
3	ADP	B	545	27/27	0.97	0.07	29,46,59,62	0
2	MG	A	544	1/1	0.97	0.05	39,39,39,39	0
4	AF3	C	546	4/4	0.98	0.07	38,38,56,61	0
2	MG	C	544	1/1	0.99	0.04	33,33,33,33	0
2	MG	B	544	1/1	0.99	0.03	39,39,39,39	0

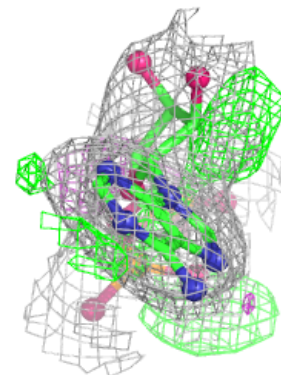
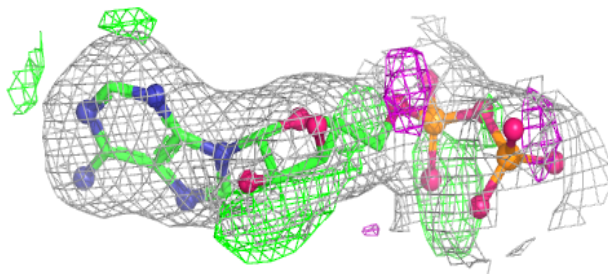
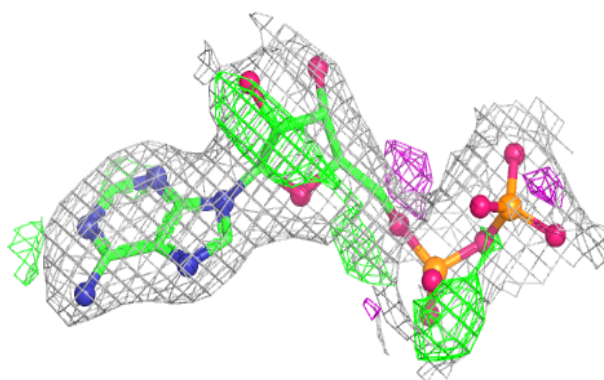
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP 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)

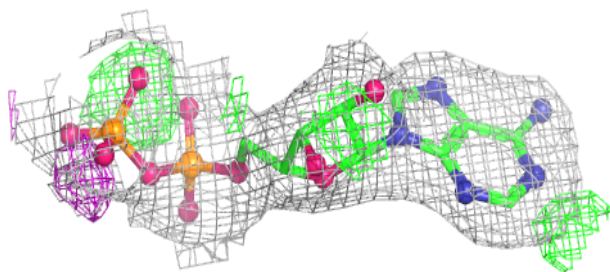
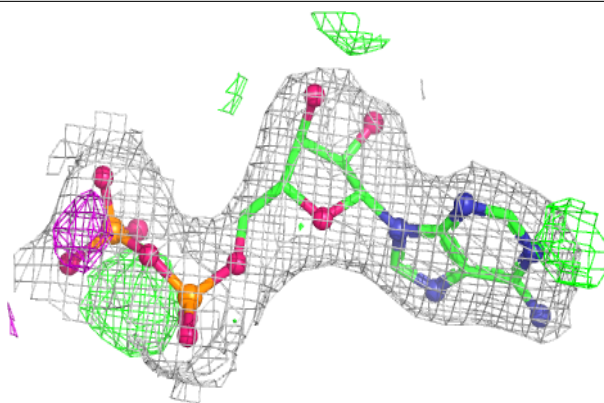
**Electron density around ADP D 545:**

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

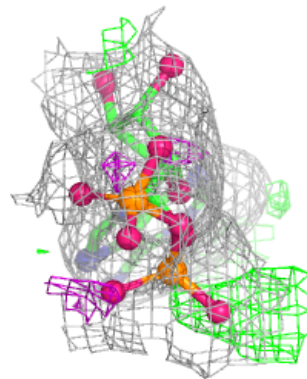
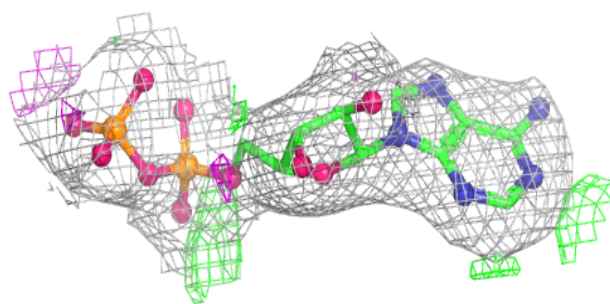
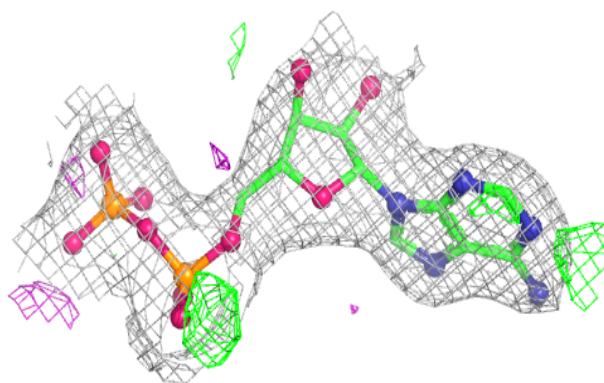


Electron density around ADP A 545:

$2mF_o-DF_c$ (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.