Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2023 – 05:35 PM EDT

PDB ID	:	3GE1
Title	:	2.7 Angstrom Crystal Structure of Glycerol Kinase (glpK) from Staphylococcus aureus in Complex with ADP and Glycerol
Authors	:	Minasov, G.; Brunzelle, J.; Skarina, T.; Onopriyenko, O.; Peterson, S.N.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2009-02-24
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 (i) 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 (1)) were used in the production of this report:

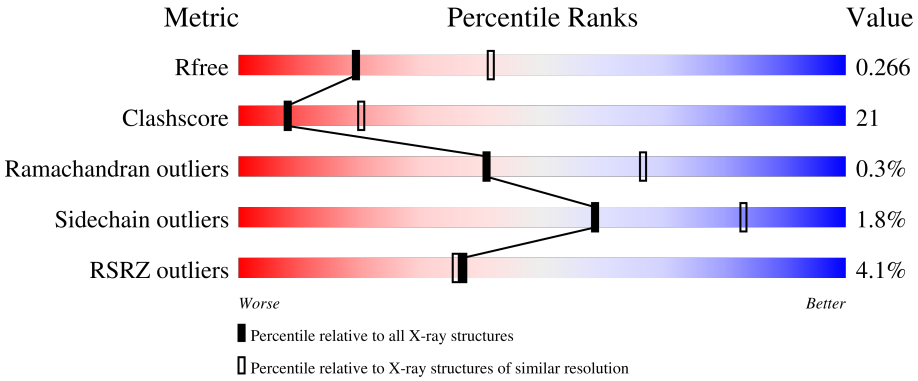
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	501	4% 66% 32% ·
1	B	501	5% 66% 33% ··
1	C	501	4% 63% 34% ··
1	D	501	3% 67% 30% ··

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16129 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.

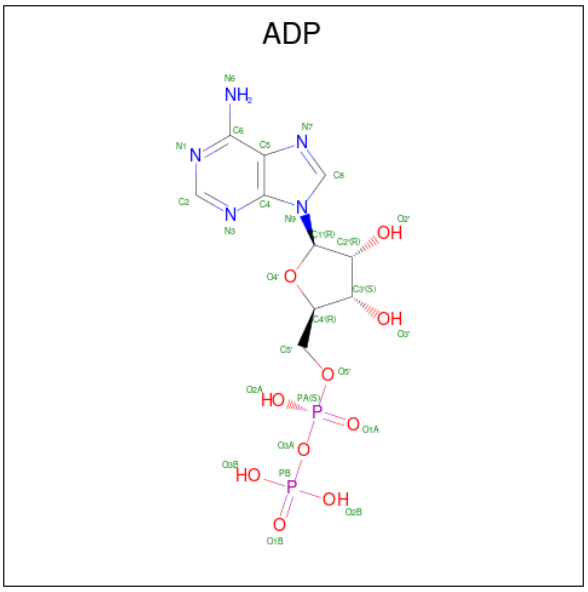
- Molecule 1 is a protein called Glycerol kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	Se	0	0	0
			3927	2485	662	766	3	11			
1	B	498	Total	C	N	O	S	Se	0	0	0
			3917	2480	661	762	3	11			
1	C	497	Total	C	N	O	S	Se	0	1	0
			3921	2482	661	764	3	11			
1	D	496	Total	C	N	O	S	Se	0	1	0
			3913	2477	660	763	3	10			

There are 12 discrepancies between the modelled and reference sequences:

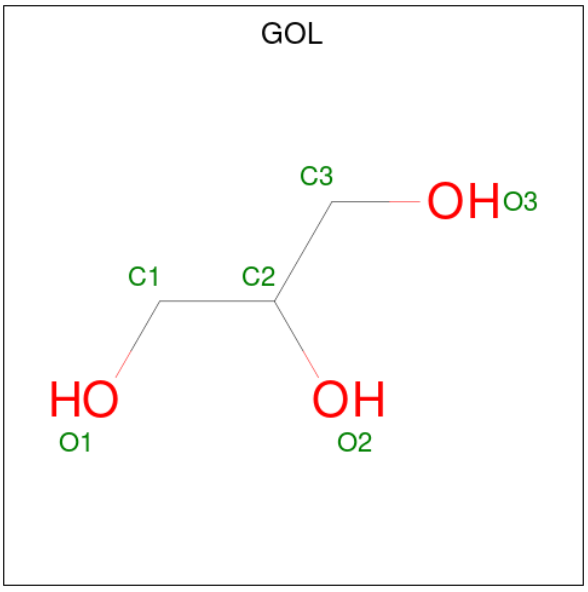
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5HGD2
A	-1	ASN	-	expression tag	UNP Q5HGD2
A	0	ALA	-	expression tag	UNP Q5HGD2
B	-2	SER	-	expression tag	UNP Q5HGD2
B	-1	ASN	-	expression tag	UNP Q5HGD2
B	0	ALA	-	expression tag	UNP Q5HGD2
C	-2	SER	-	expression tag	UNP Q5HGD2
C	-1	ASN	-	expression tag	UNP Q5HGD2
C	0	ALA	-	expression tag	UNP Q5HGD2
D	-2	SER	-	expression tag	UNP Q5HGD2
D	-1	ASN	-	expression tag	UNP Q5HGD2
D	0	ALA	-	expression tag	UNP Q5HGD2

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



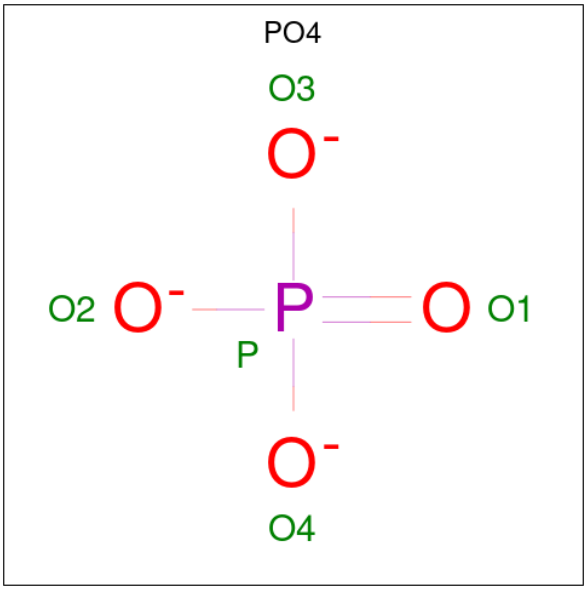
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is water.

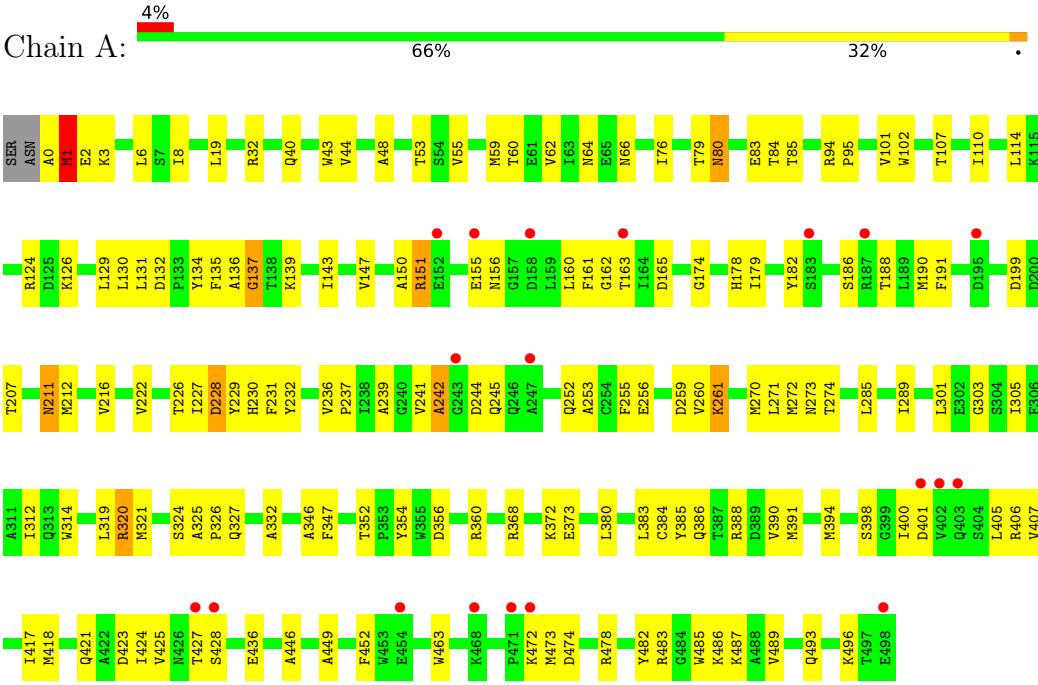
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	82	Total O 82 82	0	0
6	B	67	Total O 67 67	0	0
6	C	52	Total O 52 52	0	0
6	D	73	Total O 74 74	0	1

3 Residue-property plots (i)

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

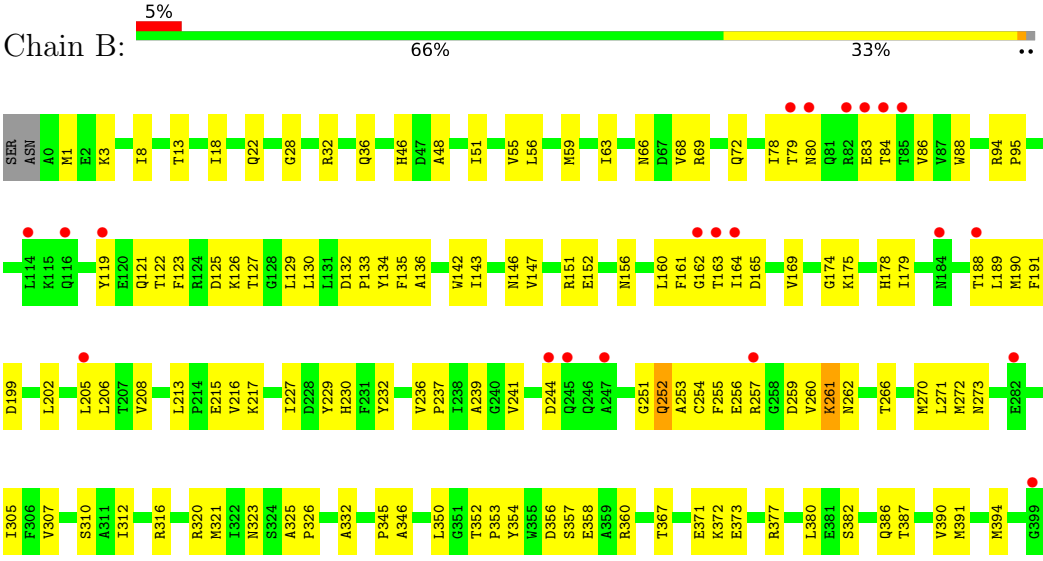
- Molecule 1: Glycerol kinase

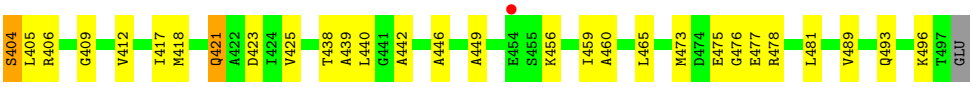
Chain A:



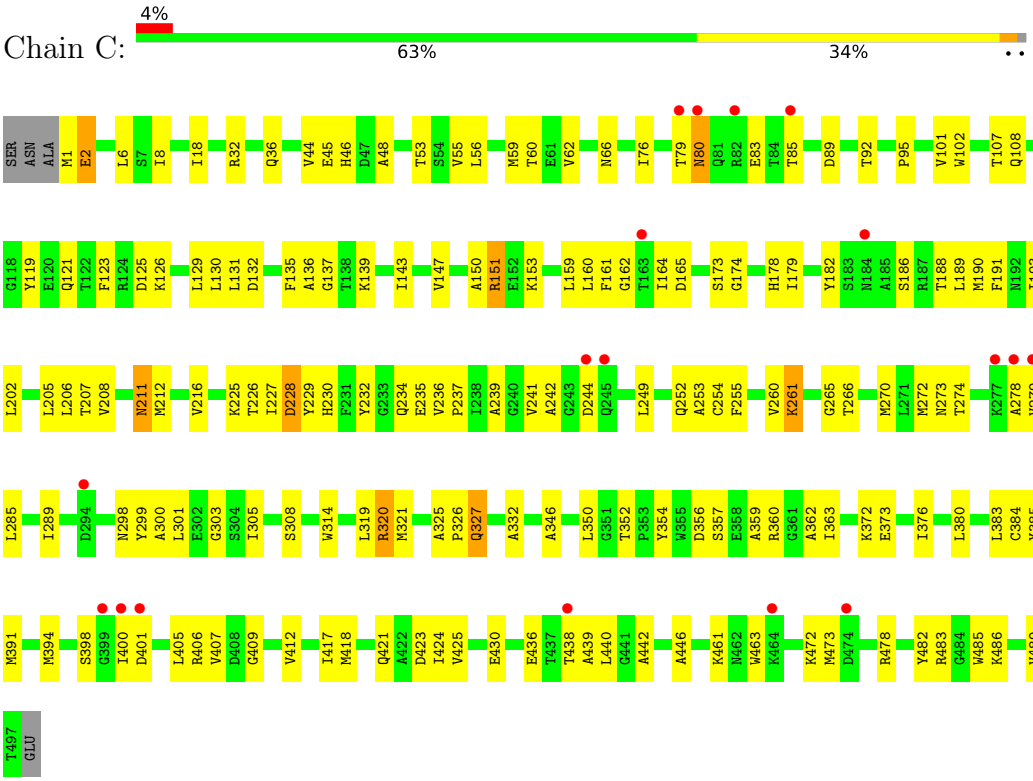
- Molecule 1: Glycerol kinase

Chain B:

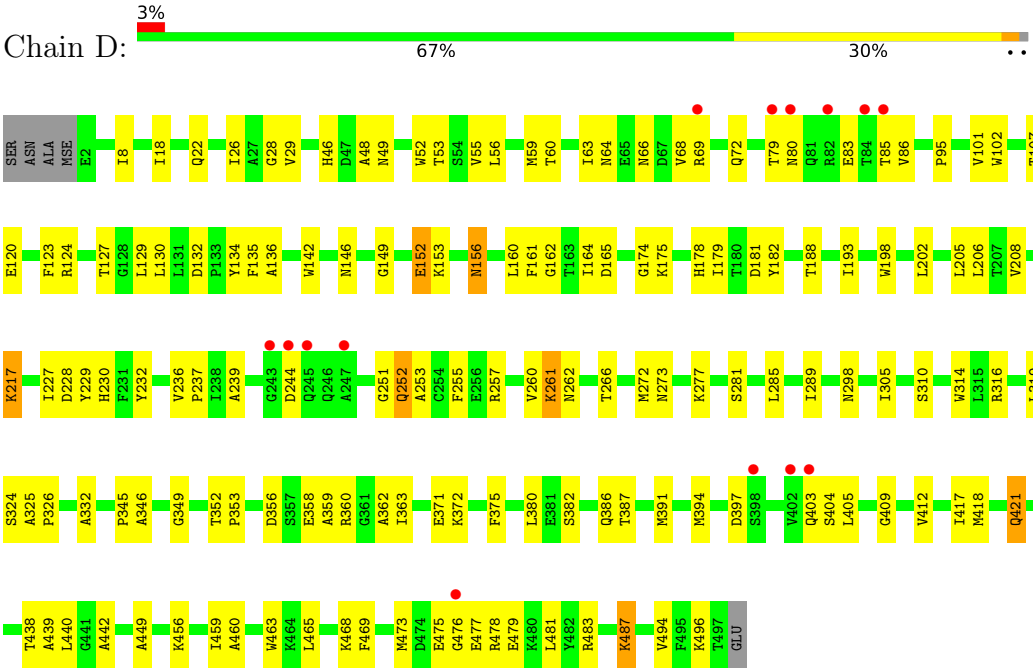




• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.41Å 193.65Å 91.84Å 90.00° 106.01° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-2.70) 96.8 (29.93-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.191 , 0.253 0.209 , 0.266	Depositor DCC
R_{free} test set	2855 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.936	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16129	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ADP, PO4, GOL

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	0.38	0/3997	0.55	5/5391 (0.1%)
1	B	0.38	0/3987	0.53	0/5379
1	C	0.37	0/3992	0.54	3/5387 (0.1%)
1	D	0.40	0/3984	0.54	1/5377 (0.0%)
All	All	0.38	0/15960	0.54	9/21534 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	320	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	320	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	320	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	C	483	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	483	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	368	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	320	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	483	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3927	0	3822	185	0
1	B	3917	0	3816	166	0
1	C	3921	0	3816	176	0
1	D	3913	0	3804	156	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	1	0
4	A	15	0	0	2	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	15	0	0	0	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	82	0	0	4	0
6	B	67	0	0	4	0
6	C	52	0	0	3	0
6	D	74	0	0	2	0
All	All	16129	0	15338	664	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 21.

All (664) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:CD1	1:A:59:MSE:HE3	1.29	1.58
1:C:8:ILE:CD1	1:C:59:MSE:HE3	1.33	1.56
1:A:8:ILE:HD11	1:A:59:MSE:CE	1.49	1.43
1:C:8:ILE:HD11	1:C:59:MSE:CE	1.53	1.38
1:D:473:MSE:HE1	1:D:481:LEU:HD12	1.17	1.12
1:C:407:VAL:HG21	1:C:418:MSE:CE	1.79	1.12
1:B:473:MSE:HE1	1:B:481:LEU:HD12	1.33	1.10
1:B:412:VAL:HA	1:B:418:MSE:HE3	1.35	1.08
1:C:227:ILE:HD12	1:C:229:TYR:CZ	1.92	1.03
1:A:8:ILE:HD12	1:A:59:MSE:HE3	1.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MSE:HA	6:B:552:HOH:O	1.60	1.02
1:C:321:MSE:HE2	1:C:372:LYS:HG3	1.41	1.02
1:C:407:VAL:CG2	1:C:418:MSE:HE1	1.91	0.98
1:C:1:MSE:HE2	1:C:1:MSE:HA	1.44	0.97
1:C:8:ILE:HD12	1:C:59:MSE:HE3	1.44	0.97
1:C:407:VAL:HG21	1:C:418:MSE:HE1	0.97	0.97
1:A:308:SER:OG	1:A:383:LEU:HD23	1.65	0.96
1:A:130:LEU:HD11	1:A:132:ASP:HB2	1.48	0.95
1:A:8:ILE:CD1	1:A:59:MSE:CE	2.22	0.94
1:B:456:LYS:O	1:B:459:ILE:HG22	1.67	0.94
1:C:8:ILE:CD1	1:C:59:MSE:CE	2.27	0.93
1:A:211:ASN:C	1:A:211:ASN:HD22	1.72	0.92
1:A:412:VAL:HB	1:A:418:MSE:HE2	1.50	0.92
1:C:305:ILE:HD13	1:C:386:GLN:HB3	1.51	0.91
1:A:32:ARG:HH21	1:C:32:ARG:HD3	1.36	0.89
1:C:391:MSE:HE1	1:C:405:LEU:HD22	1.55	0.89
1:B:227:ILE:HD12	1:B:229:TYR:CZ	2.08	0.88
1:C:473:MSE:HE3	1:C:478:ARG:HG3	1.53	0.88
1:A:270:MSE:HE1	1:A:391:MSE:HE3	1.54	0.88
1:C:130:LEU:HD11	1:C:132:ASP:HB2	1.54	0.88
1:A:227:ILE:HD12	1:A:229:TYR:CZ	2.09	0.88
1:C:272:MSE:HE1	1:C:398:SER:HB3	1.56	0.88
1:D:473:MSE:HE1	1:D:481:LEU:CD1	2.02	0.86
1:B:217:LYS:HE2	6:B:563:HOH:O	1.76	0.85
1:B:55:VAL:HG12	1:B:59:MSE:HE3	1.60	0.84
1:B:305:ILE:HD13	1:B:386:GLN:HB3	1.59	0.84
1:A:321:MSE:HE2	1:A:372:LYS:HG3	1.58	0.83
1:A:424:ILE:HD12	1:A:473:MSE:HE1	1.60	0.83
1:D:456:LYS:O	1:D:459:ILE:HG22	1.78	0.83
1:A:391:MSE:HE1	1:A:405:LEU:HD22	1.58	0.82
1:B:421:GLN:HE21	1:B:421:GLN:HA	1.45	0.82
1:D:473:MSE:HE2	1:D:478:ARG:HA	1.60	0.81
1:A:211:ASN:HD22	1:A:212:MSE:N	1.78	0.80
1:A:305:ILE:HD13	1:A:386:GLN:HB3	1.61	0.80
1:C:424:ILE:HD12	1:C:473:MSE:HE1	1.63	0.80
1:D:473:MSE:CE	1:D:481:LEU:HD12	2.08	0.80
1:A:412:VAL:CB	1:A:418:MSE:HE2	2.13	0.79
1:C:372:LYS:O	1:C:376:ILE:HD12	1.83	0.78
1:D:403:GLN:C	1:D:427:THR:HG23	2.06	0.76
1:D:473:MSE:HE2	1:D:478:ARG:N	2.01	0.76
1:A:227:ILE:HD11	1:A:230:HIS:HD2	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:NH2	1:C:32:ARG:HD3	2.00	0.76
1:B:119:TYR:CD2	1:B:205:LEU:HD21	2.22	0.75
1:B:473:MSE:HE1	1:B:481:LEU:CD1	2.15	0.75
1:C:321:MSE:CE	1:C:372:LYS:HG3	2.14	0.74
1:D:473:MSE:HE2	1:D:478:ARG:CA	2.17	0.74
1:D:473:MSE:HE3	1:D:477:GLU:HG2	1.70	0.74
1:C:409:GLY:O	1:C:412:VAL:HG22	1.87	0.74
1:D:255:PHE:HZ	1:D:459:ILE:HG21	1.52	0.74
1:B:358:GLU:HB2	1:B:496:LYS:HD3	1.68	0.74
1:D:130:LEU:HD11	1:D:132:ASP:HB2	1.66	0.74
1:A:8:ILE:HD11	1:A:59:MSE:HE3	0.75	0.74
1:A:130:LEU:CD1	1:A:132:ASP:HB2	2.18	0.74
1:A:174:GLY:HA3	1:A:227:ILE:HD13	1.70	0.74
1:A:285:LEU:HD23	1:A:352:THR:HG21	1.69	0.73
1:B:421:GLN:HA	1:B:421:GLN:NE2	2.03	0.73
1:C:380:LEU:HD22	1:C:417:ILE:HD11	1.70	0.73
1:C:174:GLY:HA3	1:C:227:ILE:HD13	1.69	0.73
1:C:8:ILE:HD11	1:C:59:MSE:HE3	0.76	0.73
1:D:260:VAL:HG22	1:D:272:MSE:HB2	1.71	0.73
1:C:211:ASN:C	1:C:211:ASN:HD22	1.92	0.73
1:D:421:GLN:HA	1:D:421:GLN:HE21	1.53	0.73
1:B:251:GLY:HA2	1:B:459:ILE:HD11	1.69	0.73
1:D:28:GLY:HA3	1:D:66:ASN:ND2	2.03	0.73
1:B:255:PHE:HZ	1:B:459:ILE:HG21	1.53	0.72
1:B:305:ILE:HD13	1:B:386:GLN:CB	2.18	0.72
1:D:403:GLN:O	1:D:427:THR:HG23	1.89	0.72
1:A:407:VAL:HG21	1:A:418:MSE:HE1	1.70	0.72
1:C:1:MSE:HA	1:C:1:MSE:CE	2.19	0.71
1:B:473:MSE:HE3	1:B:477:GLU:HG2	1.73	0.71
1:A:60:THR:HG22	1:C:53:THR:HG22	1.73	0.71
1:D:305:ILE:HG23	1:D:386:GLN:OE1	1.89	0.71
1:A:473:MSE:HE3	1:A:478:ARG:HG3	1.72	0.71
1:C:227:ILE:HD11	1:C:230:HIS:HD2	1.54	0.71
1:D:251:GLY:HA2	1:D:459:ILE:HD11	1.71	0.71
1:A:151:ARG:NH2	1:A:207:THR:O	2.24	0.70
1:D:391:MSE:SE	1:D:425:VAL:HG11	2.41	0.70
1:C:179:ILE:C	1:C:179:ILE:HD12	2.11	0.70
1:A:48:ALA:HB3	1:A:95:PRO:HG2	1.73	0.70
1:B:227:ILE:HD11	1:B:230:HIS:CD2	2.27	0.70
1:A:174:GLY:CA	1:A:227:ILE:HD13	2.22	0.70
1:A:79:THR:OG1	1:A:244:ASP:HA	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:MSE:HE2	1:B:478:ARG:N	2.07	0.69
1:C:18:ILE:HD12	1:C:439:ALA:CB	2.21	0.69
1:C:211:ASN:HD22	1:C:212:MSE:N	1.90	0.69
1:D:421:GLN:HA	1:D:421:GLN:NE2	2.07	0.69
1:B:129:LEU:HD13	1:B:135:PHE:CD1	2.28	0.69
1:C:174:GLY:CA	1:C:227:ILE:HD13	2.22	0.69
1:A:412:VAL:HB	1:A:418:MSE:CE	2.21	0.69
1:C:126:LYS:HD3	1:C:199:ASP:OD1	1.93	0.69
1:D:80:ASN:HD22	1:D:164:ILE:HB	1.56	0.69
1:A:179:ILE:C	1:A:179:ILE:HD12	2.13	0.69
1:D:409:GLY:O	1:D:412:VAL:HG22	1.91	0.69
1:C:227:ILE:CD1	1:C:229:TYR:CZ	2.75	0.68
1:B:48:ALA:HB3	1:B:95:PRO:HG3	1.75	0.68
1:D:285:LEU:HD11	1:D:394:MSE:HA	1.75	0.68
1:D:261:LYS:HD2	1:D:261:LYS:C	2.14	0.68
1:A:80:ASN:C	1:A:80:ASN:HD22	1.98	0.68
1:D:179:ILE:HD12	1:D:179:ILE:C	2.15	0.67
1:D:63:ILE:HD12	1:D:232:TYR:CE2	2.29	0.67
1:B:285:LEU:HD11	1:B:394:MSE:HA	1.75	0.67
1:A:407:VAL:CG2	1:A:418:MSE:HE1	2.25	0.67
1:B:130:LEU:HD11	1:B:132:ASP:HB2	1.77	0.67
1:C:80:ASN:HD22	1:C:80:ASN:C	1.97	0.67
1:A:211:ASN:C	1:A:211:ASN:ND2	2.45	0.67
1:A:409:GLY:O	1:A:412:VAL:HG22	1.95	0.67
1:B:465:LEU:C	1:B:465:LEU:HD23	2.15	0.66
1:C:79:THR:OG1	1:C:244:ASP:HA	1.96	0.66
1:B:473:MSE:HE2	1:B:477:GLU:C	2.16	0.66
1:B:198:TRP:CG	1:B:213:LEU:HD13	2.30	0.66
1:D:215[B]:GLU:HG2	1:D:217:LYS:HE3	1.75	0.66
1:B:179:ILE:HD12	1:B:179:ILE:C	2.17	0.66
1:B:380:LEU:HD22	1:B:417:ILE:HD11	1.77	0.65
1:A:151:ARG:HH11	1:A:151:ARG:CG	2.10	0.65
1:D:465:LEU:C	1:D:465:LEU:HD23	2.17	0.65
1:C:346:ALA:O	1:C:360:ARG:HA	1.95	0.65
1:A:260:VAL:HG22	1:A:272:MSE:HB2	1.78	0.65
1:A:332:ALA:HB2	1:A:380:LEU:HD12	1.79	0.65
1:A:227:ILE:HD11	1:A:230:HIS:CD2	2.31	0.64
1:A:383:LEU:HD13	1:A:417:ILE:HD13	1.79	0.64
1:A:391:MSE:CE	1:A:405:LEU:HD22	2.27	0.64
1:A:8:ILE:HD13	1:A:55:VAL:HG13	1.79	0.64
1:B:28:GLY:HA3	1:B:66:ASN:ND2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:SER:OG	1:A:383:LEU:CD2	2.45	0.64
1:A:407:VAL:HG21	1:A:418:MSE:CE	2.27	0.64
1:C:473:MSE:HE3	1:C:478:ARG:CG	2.28	0.64
1:C:48:ALA:HB3	1:C:95:PRO:HG2	1.80	0.64
1:D:156:ASN:N	1:D:156:ASN:HD22	1.94	0.64
1:C:83:GLU:HB2	1:C:102:TRP:HB3	1.80	0.64
1:C:261:LYS:C	1:C:261:LYS:HD2	2.19	0.64
1:A:191:PHE:CE2	1:A:216:VAL:HG21	2.33	0.63
1:C:227:ILE:HD12	1:C:229:TYR:CE1	2.32	0.63
1:A:272:MSE:CE	1:A:301:LEU:HD12	2.29	0.63
1:C:130:LEU:C	1:C:130:LEU:HD12	2.19	0.63
1:C:252:GLN:O	1:C:406:ARG:NH1	2.32	0.63
1:C:8:ILE:HD13	1:C:55:VAL:HG13	1.80	0.63
1:A:130:LEU:C	1:A:130:LEU:HD12	2.19	0.63
1:C:179:ILE:HD12	1:C:179:ILE:O	1.99	0.63
1:B:261:LYS:HD2	1:B:261:LYS:C	2.18	0.63
1:A:83:GLU:HB2	1:A:102:TRP:HB3	1.79	0.62
1:A:143:ILE:HG23	1:A:147:VAL:HG21	1.82	0.62
1:A:160:LEU:HD22	1:A:178:HIS:CE1	2.35	0.62
1:C:270:MSE:HE1	1:C:391:MSE:HE3	1.80	0.62
1:C:473:MSE:CE	1:C:478:ARG:HG3	2.27	0.62
1:B:346:ALA:O	1:B:360:ARG:HA	1.99	0.62
1:A:384:CYS:HA	1:A:421:GLN:OE1	1.98	0.62
1:C:191:PHE:CE2	1:C:216:VAL:HG21	2.34	0.62
1:B:440:LEU:C	1:B:440:LEU:HD23	2.20	0.62
1:C:227:ILE:HD11	1:C:230:HIS:CD2	2.34	0.62
1:B:305:ILE:HG23	1:B:386:GLN:OE1	2.00	0.61
1:B:493:GLN:O	1:B:496:LYS:HE3	2.00	0.61
1:D:459:ILE:HG23	1:D:460:ALA:N	2.15	0.61
1:B:473:MSE:HE2	1:B:478:ARG:HA	1.83	0.61
1:C:346:ALA:HB3	1:C:360:ARG:O	2.00	0.61
1:B:69:ARG:HB2	1:B:72:GLN:HG3	1.80	0.61
1:A:261:LYS:C	1:A:261:LYS:HD2	2.21	0.61
1:A:373:GLU:N	1:A:373:GLU:OE1	2.33	0.61
1:B:257:ARG:HA	1:B:273:ASN:O	1.99	0.61
1:B:22:GLN:HE21	1:B:22:GLN:HA	1.66	0.60
1:A:474:ASP:HB2	6:A:557:HOH:O	2.01	0.60
1:C:285:LEU:HD13	1:C:394:MSE:HE2	1.81	0.60
1:D:119:TYR:CD2	1:D:205:LEU:HD21	2.36	0.60
1:C:62:VAL:O	1:C:66:ASN:ND2	2.33	0.60
1:A:285:LEU:CD2	1:A:352:THR:HG21	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:TRP:CE2	1:B:146:ASN:ND2	2.69	0.60
1:D:130:LEU:C	1:D:130:LEU:HD12	2.22	0.60
1:D:346:ALA:O	1:D:360:ARG:HA	2.01	0.60
1:A:6:LEU:HD21	1:A:59:MSE:HG2	1.84	0.59
1:B:152:GLU:CD	1:B:152:GLU:H	2.05	0.59
1:A:151:ARG:HH11	1:A:151:ARG:HG3	1.68	0.59
1:B:227:ILE:CD1	1:B:229:TYR:CZ	2.85	0.59
1:A:436:GLU:OE2	1:A:436:GLU:N	2.35	0.59
1:A:110:ILE:HG13	6:A:521:HOH:O	2.03	0.59
1:A:380:LEU:HD22	1:A:417:ILE:HD11	1.85	0.59
1:B:8:ILE:CD1	1:B:59:MSE:HE2	2.32	0.59
1:A:321:MSE:CE	1:A:372:LYS:HG3	2.31	0.59
1:C:308:SER:OG	1:C:383:LEU:HD23	2.03	0.59
1:C:174:GLY:HA3	1:C:227:ILE:HG21	1.85	0.58
1:A:126:LYS:HD3	1:A:199:ASP:OD1	2.03	0.58
1:D:473:MSE:CE	1:D:478:ARG:HA	2.30	0.58
1:A:487:LYS:HG2	6:A:527:HOH:O	2.03	0.58
1:C:239:ALA:O	1:C:446:ALA:HA	2.04	0.58
1:A:391:MSE:SE	1:A:425:VAL:HG11	2.54	0.58
1:B:80:ASN:HD22	1:B:164:ILE:HB	1.69	0.58
1:D:48:ALA:HB3	1:D:95:PRO:HG3	1.84	0.58
1:A:129:LEU:HD13	1:A:135:PHE:CD1	2.37	0.58
1:B:272:MSE:HE2	1:B:301:LEU:HD12	1.86	0.58
1:B:252:GLN:O	1:B:253:ALA:HB3	2.04	0.58
1:B:391:MSE:SE	1:B:425:VAL:HG11	2.53	0.58
1:B:130:LEU:HD12	1:B:130:LEU:C	2.24	0.57
1:B:79:THR:HG21	1:B:438:THR:HG22	1.85	0.57
1:B:227:ILE:HD11	1:B:230:HIS:HD2	1.69	0.57
1:A:373:GLU:OE1	1:B:320:ARG:NH1	2.36	0.57
1:A:252:GLN:O	1:A:406:ARG:NH1	2.38	0.57
1:A:211:ASN:ND2	1:A:212:MSE:N	2.51	0.57
1:D:440:LEU:C	1:D:440:LEU:HD23	2.24	0.57
1:A:161:PHE:CG	1:A:162:GLY:N	2.72	0.57
1:A:236:VAL:HG13	1:A:237:PRO:HD2	1.87	0.57
1:D:179:ILE:HG22	1:D:215[A]:GLU:HB2	1.87	0.57
1:D:79:THR:HG21	1:D:438:THR:HG22	1.86	0.56
1:A:32:ARG:HH21	1:C:32:ARG:CD	2.15	0.56
1:C:130:LEU:CD1	1:C:132:ASP:HB2	2.31	0.56
1:C:160:LEU:HD22	1:C:178:HIS:CE1	2.41	0.56
1:C:260:VAL:HG22	1:C:272:MSE:HB2	1.87	0.56
1:D:123:PHE:CE2	1:D:202:LEU:HD22	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:MSE:HE3	1:D:477:GLU:CG	2.35	0.56
1:B:161:PHE:CG	1:B:162:GLY:N	2.74	0.56
1:B:409:GLY:O	1:B:412:VAL:HG22	2.06	0.56
1:C:321:MSE:HE2	1:C:372:LYS:CG	2.26	0.56
1:C:354:TYR:CZ	1:C:489:VAL:HG11	2.41	0.56
1:D:179:ILE:HD12	1:D:179:ILE:O	2.06	0.56
1:A:473:MSE:HE3	1:A:478:ARG:HA	1.87	0.56
1:B:18:ILE:HD12	1:B:439:ALA:CB	2.36	0.56
1:C:436:GLU:OE2	1:C:436:GLU:N	2.38	0.56
1:B:285:LEU:HD11	1:B:394:MSE:CA	2.36	0.55
1:C:44:VAL:HG12	1:C:101:VAL:HG21	1.87	0.55
1:D:66:ASN:O	1:D:68:VAL:HG23	2.06	0.55
1:B:127:THR:O	1:B:193:ILE:HD13	2.06	0.55
1:B:473:MSE:HE2	1:B:478:ARG:CA	2.36	0.55
1:D:206:LEU:O	1:D:208:VAL:HG23	2.07	0.55
1:C:121:GLN:NE2	1:C:125:ASP:OD1	2.40	0.55
1:C:186:SER:HB3	1:C:289:ILE:HD13	1.87	0.55
1:B:473:MSE:CE	1:B:481:LEU:HD12	2.23	0.55
1:C:151:ARG:NH2	1:C:207:THR:O	2.40	0.55
1:D:129:LEU:HD13	1:D:135:PHE:CD1	2.42	0.55
1:D:130:LEU:CD1	1:D:132:ASP:HB2	2.37	0.55
1:C:279:VAL:HG22	6:C:520:HOH:O	2.06	0.55
1:D:69:ARG:HB2	1:D:72:GLN:HG3	1.87	0.55
1:D:473:MSE:HE2	1:D:477:GLU:C	2.26	0.55
1:A:60:THR:HG21	1:C:56:LEU:HD23	1.89	0.55
1:D:8:ILE:HD11	1:D:59:MSE:SE	2.57	0.55
1:B:130:LEU:CD1	1:B:132:ASP:HB2	2.37	0.55
1:C:391:MSE:SE	1:C:425:VAL:HG11	2.56	0.55
1:D:227:ILE:HD11	1:D:230:HIS:CD2	2.41	0.55
1:C:236:VAL:HG13	1:C:237:PRO:HD2	1.89	0.54
1:D:380:LEU:HD22	1:D:417:ILE:HD11	1.89	0.54
1:A:53:THR:HG22	1:C:60:THR:HG22	1.88	0.54
1:C:136:ALA:HB3	1:C:188:THR:HA	1.89	0.54
1:C:161:PHE:CG	1:C:162:GLY:N	2.75	0.54
1:C:190:MSE:HG2	1:C:206:LEU:HD12	1.89	0.54
1:D:79:THR:HB	1:D:442:ALA:HB2	1.89	0.54
1:D:179:ILE:HG22	1:D:215[B]:GLU:HB3	1.89	0.54
1:A:62:VAL:O	1:A:66:ASN:ND2	2.39	0.54
1:D:387:THR:HB	1:D:421:GLN:OE1	2.07	0.54
1:B:387:THR:O	1:B:390:VAL:HG22	2.07	0.54
1:D:421:GLN:HE21	1:D:421:GLN:CA	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASN:O	1:B:68:VAL:HG23	2.06	0.54
1:B:260:VAL:HG22	1:B:272:MSE:HB2	1.89	0.54
1:A:373:GLU:CD	1:B:320:ARG:HH12	2.12	0.53
1:B:156:ASN:N	1:B:156:ASN:HD22	2.04	0.53
1:C:129:LEU:HD13	1:C:135:PHE:CD1	2.43	0.53
1:C:391:MSE:CE	1:C:405:LEU:HD22	2.35	0.53
1:A:423:ASP:O	1:A:478:ARG:NH1	2.41	0.53
1:D:60:THR:HA	1:D:232:TYR:OH	2.09	0.53
1:A:256:GLU:CD	1:A:259:ASP:OD1	2.47	0.53
1:D:332:ALA:HB2	1:D:380:LEU:HD12	1.90	0.53
1:A:356:ASP:OD2	1:A:496:LYS:NZ	2.34	0.53
1:B:56:LEU:HD23	1:D:60:THR:HG21	1.89	0.53
1:B:371:GLU:O	1:B:372:LYS:C	2.47	0.53
1:D:174:GLY:CA	1:D:227:ILE:HD13	2.39	0.53
1:D:252:GLN:O	1:D:253:ALA:HB3	2.08	0.53
1:A:174:GLY:HA3	1:A:227:ILE:HG21	1.90	0.53
1:B:80:ASN:ND2	1:B:165:ASP:H	2.07	0.53
1:B:356:ASP:OD2	1:B:496:LYS:NZ	2.40	0.53
1:D:152:GLU:CD	1:D:152:GLU:H	2.12	0.53
1:D:257:ARG:HA	1:D:273:ASN:O	2.08	0.53
1:B:251:GLY:CA	1:B:459:ILE:HD11	2.38	0.53
1:B:473:MSE:HE3	1:B:477:GLU:CG	2.38	0.53
1:D:179:ILE:C	1:D:179:ILE:CD1	2.78	0.52
1:D:255:PHE:CZ	1:D:459:ILE:HG21	2.39	0.52
1:C:115:LYS:NZ	6:C:523:HOH:O	2.37	0.52
1:C:211:ASN:C	1:C:211:ASN:ND2	2.63	0.52
1:A:285:LEU:HD11	1:A:394:MSE:CA	2.40	0.52
1:D:266:THR:HG23	1:D:310:SER:HB2	1.91	0.52
1:B:94:ARG:NH2	1:D:64:ASN:O	2.42	0.52
1:C:424:ILE:HA	1:C:473:MSE:CE	2.39	0.52
1:D:18:ILE:HD12	1:D:439:ALA:CB	2.39	0.52
1:B:473:MSE:CE	1:B:477:GLU:HG2	2.39	0.52
1:C:179:ILE:C	1:C:179:ILE:CD1	2.78	0.52
1:D:459:ILE:CG2	1:D:460:ALA:N	2.72	0.52
1:A:285:LEU:HD13	1:A:394:MSE:HE2	1.90	0.52
1:A:190:MSE:HG2	1:A:206:LEU:HD12	1.91	0.52
1:B:421:GLN:HE21	1:B:421:GLN:CA	2.17	0.52
1:B:459:ILE:HG23	1:B:460:ALA:N	2.24	0.52
1:D:483:ARG:O	1:D:487:LYS:HD2	2.10	0.52
1:D:149:GLY:O	1:D:153:LYS:HG3	2.09	0.52
1:A:155:GLU:C	1:A:156:ASN:HD22	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:SER:HB2	1:A:327:GLN:HG3	1.92	0.52
1:B:130:LEU:HD11	1:B:132:ASP:CB	2.38	0.52
1:C:325:ALA:N	1:C:326:PRO:HD2	2.25	0.52
1:D:358:GLU:OE2	1:D:358:GLU:HA	2.10	0.52
1:B:63:ILE:HG23	1:B:68:VAL:O	2.09	0.51
1:D:101:VAL:HG12	1:D:102:TRP:N	2.25	0.51
1:A:119:TYR:CD1	1:A:205:LEU:HD21	2.45	0.51
1:B:55:VAL:CG1	1:B:59:MSE:HE3	2.37	0.51
1:D:285:LEU:HD11	1:D:394:MSE:CA	2.39	0.51
1:A:179:ILE:HD12	1:A:179:ILE:O	2.10	0.51
1:B:305:ILE:CD1	1:B:386:GLN:HB3	2.36	0.51
1:A:346:ALA:O	1:A:360:ARG:HA	2.10	0.51
1:D:22:GLN:HE21	1:D:22:GLN:HA	1.74	0.51
1:A:245:GLN:HB3	1:A:271:LEU:CD1	2.41	0.51
1:A:136:ALA:HB3	1:A:188:THR:HA	1.92	0.51
1:A:179:ILE:C	1:A:179:ILE:CD1	2.78	0.51
1:A:312:ILE:HD13	2:A:499:ADP:H2	1.75	0.51
1:C:285:LEU:HD11	1:C:394:MSE:CA	2.41	0.51
1:D:239:ALA:HB1	1:D:449:ALA:HB3	1.92	0.51
1:A:252:GLN:O	1:A:253:ALA:HB3	2.10	0.51
1:B:143:ILE:HG23	1:B:147:VAL:HG21	1.93	0.51
1:C:303:GLY:HA3	1:C:390:VAL:HG13	1.92	0.51
1:C:424:ILE:CD1	1:C:473:MSE:HE1	2.38	0.51
1:D:174:GLY:HA3	1:D:227:ILE:HD13	1.93	0.51
1:D:417:ILE:HG22	1:D:418:MSE:CE	2.41	0.51
1:A:412:VAL:CA	1:A:418:MSE:HE2	2.40	0.51
1:A:372:LYS:NZ	4:A:502:PO4:O1	2.37	0.51
1:B:206:LEU:O	1:B:208:VAL:HG23	2.11	0.51
1:D:160:LEU:HD22	1:D:178:HIS:CE1	2.46	0.50
1:B:325:ALA:HB3	1:B:326:PRO:HD3	1.92	0.50
1:D:26:ILE:HG21	1:D:29:VAL:HG23	1.93	0.50
1:D:227:ILE:HD11	1:D:230:HIS:HD2	1.75	0.50
1:D:251:GLY:CA	1:D:459:ILE:HD11	2.41	0.50
1:A:354:TYR:CZ	1:A:489:VAL:HG11	2.46	0.50
1:D:136:ALA:HB3	1:D:188:THR:HA	1.92	0.50
1:A:285:LEU:HD11	1:A:394:MSE:HA	1.93	0.50
1:B:22:GLN:HA	1:B:22:GLN:NE2	2.26	0.50
1:C:424:ILE:HA	1:C:473:MSE:HE2	1.93	0.50
1:A:163:THR:OG1	1:A:165:ASP:OD1	2.23	0.50
1:B:121:GLN:NE2	1:B:125:ASP:OD1	2.44	0.50
1:B:227:ILE:HD12	1:B:229:TYR:CE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:HG2	1:A:134:TYR:O	2.12	0.50
1:B:163:THR:OG1	1:B:165:ASP:OD1	2.20	0.50
1:B:473:MSE:CE	1:B:478:ARG:HA	2.41	0.50
1:D:161:PHE:CG	1:D:162:GLY:N	2.79	0.50
1:C:400:ILE:HG22	1:C:401:ASP:N	2.26	0.50
1:A:227:ILE:HD12	1:A:229:TYR:CE1	2.46	0.50
1:B:260:VAL:HG22	1:B:272:MSE:CB	2.42	0.50
1:C:359:ALA:O	1:C:360:ARG:NH1	2.41	0.50
1:D:63:ILE:CD1	1:D:232:TYR:CE2	2.94	0.50
1:D:281:SER:OG	1:D:397:ASP:OD2	2.23	0.50
1:A:201:GLU:HB2	6:A:547:HOH:O	2.11	0.49
1:A:325:ALA:N	1:A:326:PRO:HD2	2.27	0.49
1:B:312:ILE:HD11	1:B:380:LEU:CD2	2.42	0.49
1:C:384:CYS:HA	1:C:421:GLN:OE1	2.12	0.49
1:D:120:GLU:O	1:D:124:ARG:HG3	2.11	0.49
1:A:285:LEU:HD23	1:A:352:THR:CG2	2.40	0.49
1:B:191:PHE:CE2	1:B:216:VAL:HG21	2.47	0.49
1:C:278:ALA:HB2	1:C:299:TYR:CD1	2.48	0.49
1:D:285:LEU:HD23	1:D:352:THR:HG21	1.93	0.49
1:A:186:SER:HB3	1:A:289:ILE:HD13	1.93	0.49
1:B:79:THR:OG1	1:B:244:ASP:HA	2.13	0.49
1:D:382:SER:O	1:D:386:GLN:HG3	2.11	0.49
1:A:76:ILE:HD12	1:A:226:THR:CG2	2.42	0.49
1:A:473:MSE:HE3	1:A:478:ARG:CG	2.41	0.49
1:B:236:VAL:HG13	1:B:237:PRO:HD2	1.93	0.49
1:B:239:ALA:HB1	1:B:449:ALA:HB3	1.95	0.49
1:B:132:ASP:C	1:B:134:TYR:H	2.15	0.49
1:D:252:GLN:HE22	1:D:463:TRP:HE1	1.59	0.49
1:B:307:VAL:HG13	1:B:310:SER:HB3	1.95	0.49
1:C:325:ALA:HB3	1:C:326:PRO:HD3	1.94	0.49
1:A:0:ALA:O	1:A:1:MSE:CG	2.61	0.49
1:A:44:VAL:HG12	1:A:101:VAL:HG21	1.95	0.49
1:B:160:LEU:HD22	1:B:178:HIS:CE1	2.48	0.49
1:B:358:GLU:CB	1:B:496:LYS:HD3	2.40	0.49
1:A:80:ASN:C	1:A:80:ASN:ND2	2.65	0.49
1:D:475:GLU:O	1:D:476:GLY:C	2.51	0.49
1:A:424:ILE:HA	1:A:473:MSE:CE	2.43	0.49
1:A:3:LYS:HB2	1:A:452:PHE:HE1	1.77	0.48
1:A:76:ILE:HD12	1:A:226:THR:HG21	1.95	0.48
1:C:482:TYR:O	1:C:486:LYS:HG3	2.13	0.48
1:A:424:ILE:CD1	1:A:473:MSE:HE1	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASN:ND2	1:C:212:MSE:N	2.59	0.48
1:C:356:ASP:OD2	1:C:496:LYS:NZ	2.38	0.48
1:B:262:ASN:HB2	1:B:405:LEU:HD21	1.94	0.48
1:C:285:LEU:HD11	1:C:394:MSE:HA	1.94	0.48
1:D:49:ASN:O	1:D:53:THR:HG23	2.13	0.48
1:D:305:ILE:HD13	1:D:386:GLN:CB	2.43	0.48
1:D:305:ILE:HD13	1:D:386:GLN:HB3	1.94	0.48
1:A:0:ALA:O	1:A:1:MSE:HG2	2.13	0.48
1:D:79:THR:OG1	1:D:244:ASP:HA	2.13	0.48
1:B:179:ILE:C	1:B:179:ILE:CD1	2.81	0.48
1:C:6:LEU:HD21	1:C:59:MSE:HG2	1.95	0.48
1:D:298:ASN:N	1:D:298:ASN:HD22	2.10	0.48
1:D:325:ALA:HB3	1:D:326:PRO:HD3	1.94	0.48
1:B:136:ALA:HB3	1:B:188:THR:HA	1.94	0.48
1:C:206:LEU:O	1:C:208:VAL:HG23	2.14	0.48
1:A:312:ILE:HD11	1:A:383:LEU:HD11	1.95	0.48
1:B:475:GLU:O	1:B:476:GLY:C	2.52	0.48
1:C:261:LYS:HD2	1:C:261:LYS:O	2.13	0.48
1:C:363:ILE:O	1:D:362:ALA:HA	2.13	0.48
1:D:252:GLN:HE21	1:D:252:GLN:HA	1.79	0.48
1:B:239:ALA:O	1:B:446:ALA:HA	2.14	0.48
1:C:285:LEU:HD23	1:C:352:THR:HG21	1.96	0.48
1:A:360:ARG:HD2	1:B:367:THR:HG22	1.96	0.47
1:A:424:ILE:HA	1:A:473:MSE:HE2	1.95	0.47
1:B:188:THR:O	1:B:189:LEU:HB2	2.14	0.47
1:B:255:PHE:CZ	1:B:459:ILE:HG21	2.42	0.47
1:C:423:ASP:O	1:C:478:ARG:NH1	2.48	0.47
1:A:285:LEU:HD11	1:A:394:MSE:CB	2.44	0.47
1:A:412:VAL:HG12	1:A:418:MSE:HE1	1.96	0.47
1:A:423:ASP:OD1	1:A:472:LYS:N	2.46	0.47
1:B:126:LYS:HD3	1:B:199:ASP:OD2	2.15	0.47
1:C:80:ASN:C	1:C:80:ASN:ND2	2.66	0.47
1:D:142:TRP:CE2	1:D:146:ASN:ND2	2.80	0.47
1:A:227:ILE:CD1	1:A:229:TYR:CZ	2.92	0.47
1:A:493:GLN:O	1:A:496:LYS:HE3	2.14	0.47
1:B:83:GLU:HB2	1:B:102:TRP:HB3	1.96	0.47
1:C:319:LEU:O	1:C:320:ARG:C	2.51	0.47
1:A:485:TRP:O	1:A:489:VAL:HG23	2.13	0.47
1:C:325:ALA:HB3	1:C:326:PRO:CD	2.44	0.47
1:D:102:TRP:CE2	3:D:500:GOL:H11	2.49	0.47
1:B:79:THR:HB	1:B:442:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:HB	1:C:289:ILE:HD11	1.97	0.47
1:C:274:THR:HG23	1:C:300:ALA:HA	1.95	0.47
1:D:323:ASN:OD1	1:D:324:SER:N	2.48	0.47
1:D:428:SER:HA	1:D:469:PHE:O	2.15	0.47
1:B:179:ILE:HD12	1:B:179:ILE:O	2.14	0.47
1:A:285:LEU:HD11	1:A:394:MSE:HB2	1.97	0.47
1:A:325:ALA:HB3	1:A:326:PRO:HD3	1.97	0.47
1:C:387:THR:HB	1:C:421:GLN:HE22	1.80	0.47
1:D:314:TRP:CH2	1:D:319:LEU:HD11	2.50	0.47
1:B:101:VAL:HG12	1:B:102:TRP:N	2.29	0.46
1:A:388:ARG:HD3	1:A:482:TYR:CE1	2.49	0.46
1:C:36:GLN:OE1	1:C:46:HIS:NE2	2.41	0.46
1:C:44:VAL:HG12	1:C:101:VAL:CG2	2.46	0.46
1:C:85:THR:HG23	1:C:161:PHE:CE1	2.51	0.46
1:C:130:LEU:HD12	1:C:132:ASP:N	2.31	0.46
1:D:22:GLN:HA	1:D:22:GLN:NE2	2.30	0.46
1:A:473:MSE:CE	1:A:478:ARG:HA	2.45	0.46
1:B:119:TYR:CG	1:B:205:LEU:HD21	2.50	0.46
1:C:252:GLN:O	1:C:253:ALA:HB3	2.14	0.46
1:D:198:TRP:CG	1:D:213:LEU:HD13	2.50	0.46
1:D:356:ASP:OD2	1:D:496:LYS:NZ	2.37	0.46
1:C:188:THR:O	1:C:189:LEU:CB	2.63	0.46
1:B:55:VAL:O	1:B:59:MSE:HG3	2.16	0.46
1:A:120:GLU:O	1:A:124:ARG:HG3	2.15	0.46
1:B:262:ASN:CB	1:B:405:LEU:HD21	2.45	0.46
1:B:345:PRO:HG2	1:B:386:GLN:HE22	1.80	0.46
1:C:60:THR:HA	1:C:232:TYR:OH	2.15	0.46
1:C:79:THR:HB	1:C:442:ALA:HB2	1.97	0.46
1:A:325:ALA:HB3	1:A:326:PRO:CD	2.46	0.46
1:B:266:THR:HG23	1:B:310:SER:HB2	1.97	0.46
1:B:354:TYR:CZ	1:B:489:VAL:HG11	2.51	0.46
1:D:80:ASN:ND2	1:D:165:ASP:H	2.13	0.46
1:C:173:SER:O	1:C:227:ILE:HG23	2.15	0.46
1:C:225:LYS:HD3	1:C:235:GLU:O	2.16	0.46
1:D:262:ASN:HB2	1:D:405:LEU:HD21	1.96	0.46
1:A:473:MSE:CE	1:A:478:ARG:HG3	2.45	0.45
1:D:156:ASN:N	1:D:156:ASN:ND2	2.63	0.45
1:D:473:MSE:CE	1:D:481:LEU:CD1	2.82	0.45
1:C:89:ASP:HB3	1:C:92:THR:OG1	2.15	0.45
1:C:332:ALA:HB2	1:C:380:LEU:HD12	1.98	0.45
1:A:388:ARG:HD3	1:A:482:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLN:O	1:B:406:ARG:NH1	2.49	0.45
1:C:272:MSE:CE	1:C:301:LEU:HD12	2.47	0.45
1:C:303:GLY:HA3	1:C:390:VAL:CG1	2.47	0.45
1:A:32:ARG:HE	1:C:32:ARG:NH2	2.15	0.45
1:A:201:GLU:O	1:A:205:LEU:HD13	2.17	0.45
1:C:228:ASP:HA	1:C:234:GLN:O	2.16	0.45
1:D:181:ASP:HA	1:D:217:LYS:O	2.16	0.45
1:D:227:ILE:HD12	1:D:229:TYR:CZ	2.52	0.45
1:B:179:ILE:HG22	1:B:215:GLU:HB2	1.97	0.45
1:B:459:ILE:CG2	1:B:460:ALA:N	2.78	0.45
1:C:346:ALA:HB2	1:C:350:LEU:HD21	1.98	0.45
1:D:325:ALA:N	1:D:326:PRO:CD	2.79	0.45
1:B:198:TRP:CD2	1:B:213:LEU:HD13	2.51	0.45
1:C:45:GLU:HA	1:C:101:VAL:HG23	1.98	0.45
1:D:277:LYS:HB3	6:D:521:HOH:O	2.16	0.45
1:A:436:GLU:H	1:A:436:GLU:CD	2.19	0.45
1:C:298:ASN:HD22	1:C:298:ASN:N	2.15	0.45
1:D:130:LEU:HD11	1:D:132:ASP:CB	2.40	0.45
1:A:101:VAL:HG12	1:A:102:TRP:N	2.32	0.45
1:C:385:TYR:HB3	1:C:485:TRP:CD2	2.52	0.45
1:D:55:VAL:HG12	1:D:59:MSE:HE2	1.98	0.45
1:A:241:VAL:O	1:A:242:ALA:HB2	2.17	0.45
1:A:270:MSE:HE1	1:A:391:MSE:CE	2.36	0.45
1:D:182:TYR:HB3	1:D:289:ILE:HG21	1.99	0.45
1:C:117:GLN:HB3	1:C:119:TYR:HE2	1.82	0.45
1:D:215[B]:GLU:CG	1:D:217:LYS:HE3	2.44	0.45
1:B:123:PHE:CE2	1:B:202:LEU:HD22	2.52	0.44
1:C:130:LEU:HD12	1:C:131:LEU:N	2.31	0.44
1:C:494:VAL:HG21	1:D:494:VAL:HG21	1.99	0.44
1:D:305:ILE:CG2	1:D:386:GLN:OE1	2.61	0.44
1:D:478:ARG:HD2	1:D:479:GLU:OE2	2.17	0.44
1:A:114:LEU:HB2	1:A:131:LEU:HD13	1.98	0.44
1:A:314:TRP:CH2	1:A:319:LEU:HD11	2.51	0.44
1:B:83:GLU:O	1:B:84:THR:C	2.56	0.44
1:C:107:THR:HG21	1:C:139:LYS:HA	1.98	0.44
1:A:126:LYS:NZ	1:A:201:GLU:OE2	2.40	0.44
1:B:1:MSE:CG	1:B:1:MSE:O	2.64	0.44
1:B:305:ILE:HD13	1:B:386:GLN:HB2	1.99	0.44
1:C:285:LEU:CD2	1:C:352:THR:HG21	2.47	0.44
1:C:314:TRP:CH2	1:C:319:LEU:HD11	2.53	0.44
1:C:425:VAL:O	1:C:425:VAL:CG1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:THR:HG22	1:A:428:SER:N	2.33	0.44
1:C:346:ALA:HB3	1:C:360:ARG:C	2.38	0.44
1:D:363:ILE:HD13	1:D:375:PHE:CE1	2.52	0.44
1:B:1:MSE:O	1:B:1:MSE:HG3	2.17	0.44
1:C:201:GLU:O	1:C:205:LEU:HD13	2.17	0.44
1:C:398:SER:C	1:C:400:ILE:H	2.21	0.44
1:B:321:MSE:CE	1:B:372:LYS:HG2	2.48	0.44
1:C:147:VAL:HB	1:C:150:ALA:HB2	2.00	0.44
1:C:473:MSE:HE3	1:C:478:ARG:CB	2.47	0.44
1:A:272:MSE:HE1	1:A:301:LEU:HD12	1.98	0.44
1:D:261:LYS:C	1:D:261:LYS:CD	2.85	0.44
1:A:228:ASP:OD1	1:A:228:ASP:N	2.50	0.44
1:C:119:TYR:CD1	1:C:205:LEU:HD21	2.52	0.44
1:C:153:LYS:HE2	1:C:159:LEU:HD21	2.00	0.44
1:D:404:SER:HA	1:D:428:SER:O	2.18	0.44
1:A:245:GLN:HB3	1:A:271:LEU:HD11	1.99	0.44
1:B:78:ILE:HD12	1:B:169:VAL:HG22	1.99	0.44
1:B:129:LEU:HD13	1:B:135:PHE:CE1	2.53	0.44
1:A:303:GLY:HA3	1:A:390:VAL:HG13	2.00	0.43
1:B:316:ARG:O	1:B:320:ARG:HA	2.18	0.43
1:B:352:THR:HG22	1:B:390:VAL:HG12	1.99	0.43
1:C:101:VAL:HG12	1:C:102:TRP:N	2.33	0.43
1:C:108:GLN:OE1	1:C:357:SER:HB3	2.18	0.43
1:D:345:PRO:HG2	1:D:386:GLN:HE22	1.82	0.43
1:B:217:LYS:HD2	6:B:550:HOH:O	2.18	0.43
1:B:423:ASP:O	1:B:478:ARG:NH1	2.51	0.43
1:C:255:PHE:O	1:C:273:ASN:ND2	2.51	0.43
1:A:259:ASP:O	1:A:272:MSE:HA	2.18	0.43
1:B:51:ILE:O	1:B:55:VAL:HG23	2.19	0.43
1:B:78:ILE:O	1:B:241:VAL:HA	2.18	0.43
1:B:352:THR:HA	1:B:353:PRO:HA	1.75	0.43
1:D:63:ILE:HG23	1:D:68:VAL:O	2.18	0.43
1:A:412:VAL:CB	1:A:418:MSE:CE	2.87	0.43
1:B:325:ALA:N	1:B:326:PRO:CD	2.81	0.43
1:D:86:VAL:HA	6:D:536:HOH:O	2.19	0.43
1:D:316:ARG:O	1:D:320:ARG:HA	2.18	0.43
1:D:403:GLN:C	1:D:427:THR:CG2	2.81	0.43
1:D:418:MSE:HE2	1:D:418:MSE:HA	1.99	0.43
1:A:85:THR:HG23	1:A:161:PHE:CE1	2.54	0.43
1:B:8:ILE:HD11	1:B:59:MSE:HE2	2.00	0.43
1:B:440:LEU:HD23	1:B:440:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:HA	1:D:59:MSE:HE3	1.99	0.43
1:B:32:ARG:HA	1:B:32:ARG:HD3	1.87	0.43
1:B:440:LEU:HD21	1:B:459:ILE:HG13	2.01	0.43
1:C:76:ILE:HD12	1:C:226:THR:CG2	2.49	0.43
1:C:485:TRP:O	1:C:489:VAL:HG23	2.18	0.43
1:D:257:ARG:NH1	1:D:277:LYS:HG3	2.34	0.43
1:A:307:VAL:HG11	1:A:347:PHE:CD1	2.53	0.43
1:A:307:VAL:HG13	1:A:310:SER:HB3	1.99	0.43
1:D:107:THR:HG22	1:D:142:TRP:HB2	2.00	0.43
1:A:312:ILE:HD13	2:A:499:ADP:C2	2.53	0.43
1:A:482:TYR:O	1:A:486:LYS:HG3	2.19	0.43
1:B:312:ILE:CD1	2:B:499:ADP:C2	3.02	0.43
1:A:320:ARG:HH11	4:A:501:PO4:P	2.41	0.42
1:B:86:VAL:HG12	1:B:88:TRP:HE3	1.84	0.42
1:C:2:GLU:H	1:C:2:GLU:HG3	1.70	0.42
1:A:76:ILE:CD1	1:A:226:THR:HG21	2.50	0.42
1:B:253:ALA:HA	1:B:255:PHE:CZ	2.54	0.42
1:D:321:MSE:CE	1:D:372:LYS:HG2	2.49	0.42
1:A:119:TYR:CD1	1:A:205:LEU:CD2	3.03	0.42
1:B:229:TYR:HA	1:D:229:TYR:HA	2.02	0.42
1:B:346:ALA:HB2	1:B:350:LEU:HD21	2.01	0.42
1:C:123:PHE:CE2	1:C:202:LEU:HD22	2.54	0.42
1:C:241:VAL:O	1:C:242:ALA:HB2	2.19	0.42
1:A:151:ARG:CG	1:A:151:ARG:NH1	2.73	0.42
1:A:425:VAL:O	1:A:425:VAL:CG1	2.67	0.42
1:B:323:ASN:HB3	6:B:529:HOH:O	2.18	0.42
1:B:312:ILE:HD12	2:B:499:ADP:C2	2.54	0.42
1:C:327:GLN:HB3	6:C:508:HOH:O	2.19	0.42
1:C:425:VAL:O	1:C:425:VAL:HG12	2.18	0.42
1:C:472:LYS:O	1:C:472:LYS:HG3	2.19	0.42
1:A:59:MSE:O	1:A:62:VAL:HG12	2.20	0.42
1:B:108:GLN:OE1	1:B:357:SER:HB3	2.19	0.42
1:C:265:GLY:O	1:C:266:THR:C	2.57	0.42
1:A:107:THR:HG21	1:A:139:LYS:HA	2.02	0.42
1:C:407:VAL:CG2	1:C:418:MSE:CE	2.71	0.42
1:A:231:PHE:C	1:A:232:TYR:CD2	2.93	0.42
1:A:272:MSE:HE3	1:A:274:THR:HG22	2.02	0.42
1:C:123:PHE:CD2	1:C:202:LEU:HD22	2.55	0.42
1:C:143:ILE:HG23	1:C:147:VAL:HG21	2.02	0.42
1:C:249:LEU:HG	1:C:254:CYS:HB2	2.02	0.42
1:D:26:ILE:CG2	1:D:29:VAL:HG23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:HB	1:B:190:MSE:CE	2.50	0.42
1:C:272:MSE:HE1	1:C:398:SER:CB	2.38	0.42
1:D:101:VAL:CG1	1:D:102:TRP:N	2.83	0.42
1:D:332:ALA:CB	1:D:380:LEU:HD12	2.50	0.42
1:A:400:ILE:HG22	1:A:401:ASP:N	2.34	0.42
1:C:119:TYR:CD1	1:C:205:LEU:CD2	3.03	0.42
1:D:261:LYS:HD2	1:D:261:LYS:O	2.20	0.42
1:A:83:GLU:O	1:A:84:THR:C	2.58	0.41
1:A:255:PHE:O	1:A:273:ASN:ND2	2.53	0.41
1:B:382:SER:O	1:B:386:GLN:HG3	2.20	0.41
1:D:262:ASN:CB	1:D:405:LEU:HD21	2.50	0.41
1:A:320:ARG:NH2	1:B:373:GLU:OE1	2.53	0.41
1:C:362:ALA:HA	1:D:363:ILE:O	2.21	0.41
1:C:423:ASP:C	1:C:473:MSE:HE2	2.41	0.41
1:B:254:CYS:CB	1:B:259:ASP:HB3	2.51	0.41
1:B:456:LYS:O	1:B:459:ILE:CG2	2.55	0.41
1:C:8:ILE:HD11	1:C:59:MSE:SE	2.66	0.41
1:D:236:VAL:HG13	1:D:237:PRO:HD2	2.01	0.41
1:A:182:TYR:CB	1:A:289:ILE:HG21	2.51	0.41
1:A:245:GLN:CB	1:A:271:LEU:HD11	2.51	0.41
1:B:465:LEU:C	1:B:465:LEU:CD2	2.86	0.41
1:D:85:THR:HG23	1:D:161:PHE:CE1	2.55	0.41
1:A:472:LYS:HG3	1:A:472:LYS:O	2.20	0.41
1:B:174:GLY:O	1:B:175:LYS:HB2	2.19	0.41
1:D:52:TRP:CH2	1:D:56:LEU:HD13	2.56	0.41
1:D:83:GLU:HB2	1:D:102:TRP:HB3	2.01	0.41
1:D:371:GLU:O	1:D:372:LYS:C	2.58	0.41
1:B:270:MSE:C	1:B:271:LEU:HD12	2.40	0.41
1:C:407:VAL:HG22	1:C:430:GLU:O	2.21	0.41
1:D:46:HIS:ND1	1:D:101:VAL:HG22	2.36	0.41
1:A:136:ALA:O	1:A:137:GLY:C	2.60	0.41
1:A:239:ALA:HB1	1:A:449:ALA:HB3	2.01	0.41
1:A:385:TYR:HB3	1:A:485:TRP:CD2	2.55	0.41
1:A:473:MSE:HE3	1:A:478:ARG:CB	2.50	0.41
1:B:13:THR:HA	1:B:36:GLN:NE2	2.36	0.41
1:B:165:ASP:O	1:B:169:VAL:HG23	2.21	0.41
1:B:332:ALA:O	1:B:377:ARG:NH1	2.54	0.41
1:C:436:GLU:H	1:C:436:GLU:CD	2.24	0.41
1:A:130:LEU:HD12	1:A:132:ASP:N	2.36	0.41
1:A:147:VAL:HB	1:A:150:ALA:HB2	2.02	0.41
1:B:321:MSE:HE3	1:B:372:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:TYR:HB3	1:C:289:ILE:HG21	2.01	0.41
1:C:188:THR:O	1:C:189:LEU:HB3	2.20	0.41
1:C:252:GLN:HE22	1:C:463:TRP:HE1	1.69	0.41
1:D:127:THR:O	1:D:193:ILE:HD13	2.21	0.41
1:D:174:GLY:O	1:D:175:LYS:HB2	2.21	0.41
1:D:352:THR:HA	1:D:353:PRO:HA	1.82	0.41
1:D:417:ILE:HG22	1:D:418:MSE:HE2	2.02	0.41
1:A:94:ARG:HA	1:A:95:PRO:HD3	1.92	0.41
1:A:239:ALA:O	1:A:446:ALA:HA	2.20	0.41
1:A:252:GLN:HE22	1:A:463:TRP:HE1	1.69	0.41
1:C:285:LEU:HD11	1:C:394:MSE:CB	2.51	0.41
1:D:468:LYS:HG2	1:D:469:PHE:N	2.36	0.41
1:A:64:ASN:N	1:A:64:ASN:HD22	2.18	0.40
1:B:63:ILE:HD12	1:B:232:TYR:CE2	2.55	0.40
1:B:130:LEU:CD1	1:B:132:ASP:CB	2.99	0.40
1:C:260:VAL:HG22	1:C:272:MSE:CB	2.51	0.40
1:D:132:ASP:C	1:D:134:TYR:H	2.25	0.40
1:A:229:TYR:HA	1:C:229:TYR:HA	2.01	0.40
1:B:239:ALA:HB1	1:B:449:ALA:CB	2.52	0.40
1:C:48:ALA:HB3	1:C:95:PRO:CG	2.49	0.40
1:D:465:LEU:C	1:D:465:LEU:CD2	2.89	0.40
1:A:19:LEU:CD1	1:A:62:VAL:HG22	2.51	0.40
1:A:40:GLN:HB2	1:A:43:TRP:CD1	2.57	0.40
1:A:260:VAL:HG22	1:A:272:MSE:CB	2.46	0.40
1:A:398:SER:C	1:A:400:ILE:H	2.24	0.40
1:B:46:HIS:ND1	1:B:101:VAL:HG22	2.36	0.40
1:B:119:TYR:O	1:B:122:THR:HB	2.22	0.40
1:C:321:MSE:HG2	1:C:372:LYS:HE3	2.04	0.40
1:D:349:GLY:HA2	1:D:359:ALA:O	2.22	0.40
1:A:222:VAL:HG22	1:A:239:ALA:HB2	2.03	0.40
1:B:252:GLN:CA	1:B:252:GLN:HE21	2.34	0.40
1:B:403:GLN:O	1:B:404:SER:HB3	2.22	0.40
1:C:114:LEU:HB2	1:C:131:LEU:HD13	2.03	0.40
1:C:165:ASP:OD1	1:C:165:ASP:N	2.54	0.40
1:C:244:ASP:O	1:C:438:THR:HG23	2.21	0.40
1:C:373:GLU:OE1	1:C:373:GLU:N	2.50	0.40
1:D:252:GLN:HE21	1:D:252:GLN:CA	2.34	0.40
1:B:229:TYR:CD2	1:D:232:TYR:HA	2.57	0.40
1:D:228:ASP:OD1	1:D:229:TYR:N	2.53	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	497/501 (99%)	466 (94%)	28 (6%)	3 (1%)	25 50
1	B	496/501 (99%)	463 (93%)	31 (6%)	2 (0%)	34 60
1	C	496/501 (99%)	461 (93%)	34 (7%)	1 (0%)	47 73
1	D	495/501 (99%)	462 (93%)	33 (7%)	0	100 100
All	All	1984/2004 (99%)	1852 (93%)	126 (6%)	6 (0%)	41 66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	404	SER
1	A	1	MSE
1	A	242	ALA
1	B	133	PRO
1	C	137	GLY
1	A	137	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	413/404 (102%)	406 (98%)	7 (2%)	60 84
1	B	412/404 (102%)	406 (98%)	6 (2%)	65 86
1	C	413/404 (102%)	403 (98%)	10 (2%)	49 77
1	D	412/404 (102%)	405 (98%)	7 (2%)	60 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1650/1616 (102%)	1620 (98%)	30 (2%)	59 83

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	2	GLU
1	A	80	ASN
1	A	151	ARG
1	A	211	ASN
1	A	228	ASP
1	A	261	LYS
1	B	3	LYS
1	B	151	ARG
1	B	252	GLN
1	B	256	GLU
1	B	261	LYS
1	B	421	GLN
1	C	2	GLU
1	C	80	ASN
1	C	151	ARG
1	C	164	ILE
1	C	211	ASN
1	C	228	ASP
1	C	261	LYS
1	C	327	GLN
1	C	440	LEU
1	C	461	LYS
1	D	152	GLU
1	D	156	ASN
1	D	217	LYS
1	D	252	GLN
1	D	261	LYS
1	D	421	GLN
1	D	487	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	156	ASN

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Mol	Chain	Res	Type
1	A	211	ASN
1	A	234	GLN
1	A	252	GLN
1	A	298	ASN
1	A	313	GLN
1	A	327	GLN
1	A	403	GLN
1	B	22	GLN
1	B	64	ASN
1	B	66	ASN
1	B	80	ASN
1	B	117	GLN
1	B	156	ASN
1	B	234	GLN
1	B	252	GLN
1	B	298	ASN
1	B	403	GLN
1	B	421	GLN
1	C	156	ASN
1	C	211	ASN
1	C	230	HIS
1	C	234	GLN
1	C	252	GLN
1	C	298	ASN
1	C	313	GLN
1	C	403	GLN
1	D	22	GLN
1	D	64	ASN
1	D	66	ASN
1	D	72	GLN
1	D	80	ASN
1	D	156	ASN
1	D	234	GLN
1	D	252	GLN
1	D	298	ASN
1	D	403	GLN

5.3.3 RNA

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 monosaccharides 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	$\#\|Z\| > 2$
2	ADP	A	499	-	24,29,29	0.95	2 (8%)	29,45,45	1.27	3 (10%)
4	PO4	D	501	-	4,4,4	0.90	0	6,6,6	0.45	0
3	GOL	C	500	-	5,5,5	0.33	0	5,5,5	0.35	0
2	ADP	D	499	-	24,29,29	0.89	1 (4%)	29,45,45	1.31	3 (10%)
4	PO4	B	501	-	4,4,4	0.81	0	6,6,6	0.45	0
4	PO4	C	501	-	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	A	503	-	4,4,4	0.91	0	6,6,6	0.39	0
2	ADP	C	499	-	24,29,29	1.05	3 (12%)	29,45,45	1.35	4 (13%)
4	PO4	D	503	-	4,4,4	0.82	0	6,6,6	0.41	0
3	GOL	D	500	-	5,5,5	0.39	0	5,5,5	0.09	0
4	PO4	D	502	-	4,4,4	0.84	0	6,6,6	0.40	0
2	ADP	B	499	-	24,29,29	0.97	2 (8%)	29,45,45	1.33	4 (13%)
4	PO4	A	502	-	4,4,4	0.79	0	6,6,6	0.53	0
3	GOL	B	500	-	5,5,5	0.42	0	5,5,5	0.22	0
3	GOL	A	500	-	5,5,5	0.32	0	5,5,5	0.28	0
4	PO4	A	501	-	4,4,4	0.85	0	6,6,6	0.58	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
2	ADP	A	499	-	-	5/12/32/32	0/3/3/3
3	GOL	C	500	-	-	0/4/4/4	-
2	ADP	D	499	-	-	1/12/32/32	0/3/3/3
2	ADP	C	499	-	-	3/12/32/32	0/3/3/3
3	GOL	D	500	-	-	0/4/4/4	-
2	ADP	B	499	-	-	1/12/32/32	0/3/3/3
3	GOL	B	500	-	-	0/4/4/4	-
3	GOL	A	500	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	499	ADP	C2-N3	2.29	1.35	1.32
2	C	499	ADP	C5-C4	2.27	1.46	1.40
2	B	499	ADP	C5-C4	2.26	1.46	1.40
2	B	499	ADP	C2-N3	2.14	1.35	1.32
2	C	499	ADP	O4'-C1'	2.13	1.44	1.41
2	A	499	ADP	C2-N3	2.07	1.35	1.32
2	D	499	ADP	C5-C4	2.03	1.46	1.40
2	A	499	ADP	C5-C4	2.00	1.46	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	499	ADP	N3-C2-N1	-3.80	122.75	128.68
2	C	499	ADP	N3-C2-N1	-3.72	122.86	128.68
2	B	499	ADP	N3-C2-N1	-3.67	122.94	128.68
2	A	499	ADP	N3-C2-N1	-3.63	123.01	128.68
2	B	499	ADP	C4-C5-N7	-2.77	106.51	109.40
2	C	499	ADP	C4-C5-N7	-2.66	106.63	109.40
2	A	499	ADP	C3'-C2'-C1'	2.65	104.97	100.98
2	C	499	ADP	C3'-C2'-C1'	2.59	104.88	100.98
2	D	499	ADP	C3'-C2'-C1'	2.59	104.87	100.98
2	C	499	ADP	PA-O3A-PB	-2.46	124.39	132.83
2	A	499	ADP	C4-C5-N7	-2.42	106.88	109.40
2	B	499	ADP	PA-O3A-PB	-2.30	124.94	132.83
2	B	499	ADP	C3'-C2'-C1'	2.13	104.19	100.98
2	D	499	ADP	PA-O3A-PB	-2.02	125.89	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	499	ADP	C5'-O5'-PA-O2A
2	A	499	ADP	C5'-O5'-PA-O3A
2	A	499	ADP	C3'-C4'-C5'-O5'
2	A	499	ADP	O4'-C4'-C5'-O5'
2	C	499	ADP	C3'-C4'-C5'-O5'
2	A	499	ADP	PB-O3A-PA-O5'
2	C	499	ADP	O4'-C4'-C5'-O5'
2	C	499	ADP	C5'-O5'-PA-O3A
2	B	499	ADP	C3'-C4'-C5'-O5'
2	D	499	ADP	C5'-O5'-PA-O1A

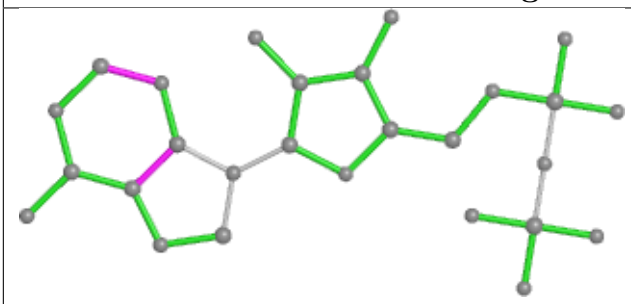
There are no ring outliers.

5 monomers are involved in 7 short contacts:

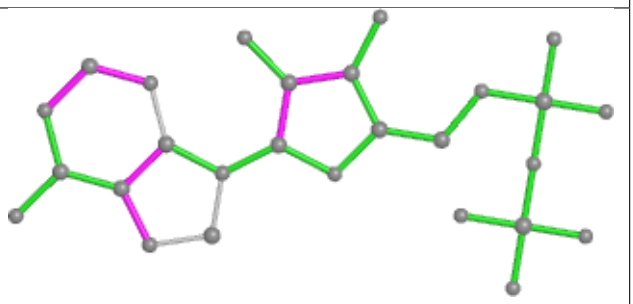
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	499	ADP	2	0
3	D	500	GOL	1	0
2	B	499	ADP	2	0
4	A	502	PO4	1	0
4	A	501	PO4	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

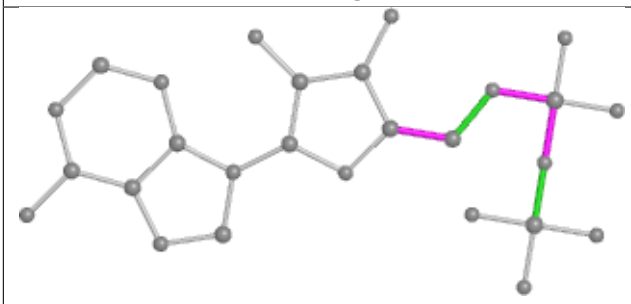
Ligand ADP A 499



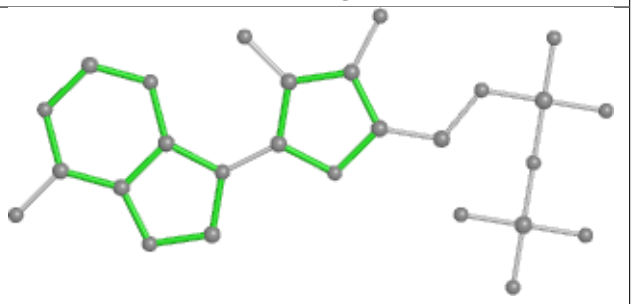
Bond lengths



Bond angles

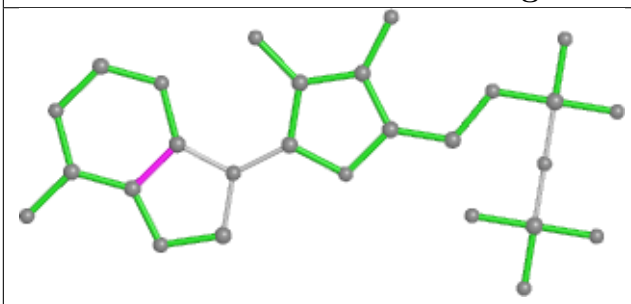


Torsions

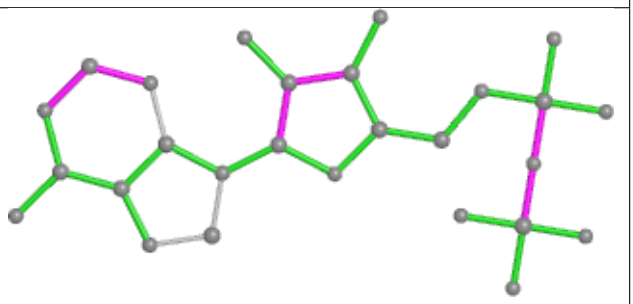


Rings

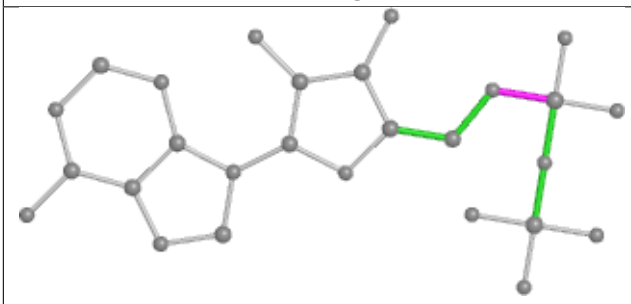
Ligand ADP D 499



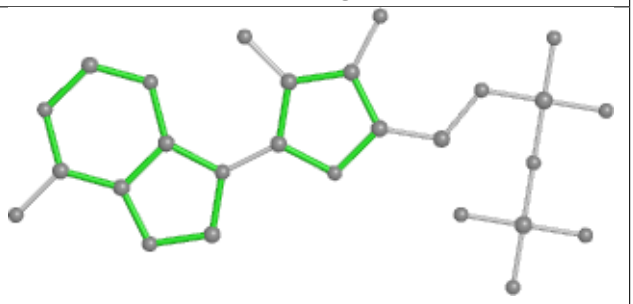
Bond lengths



Bond angles

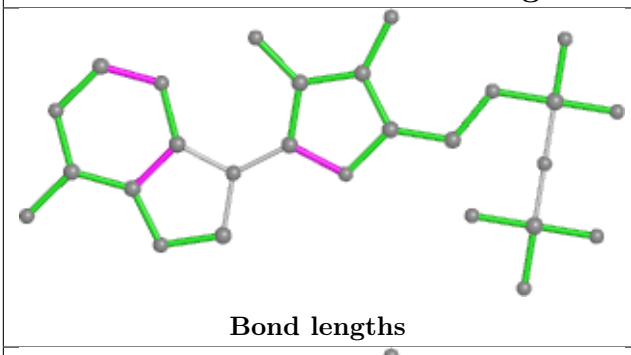


Torsions

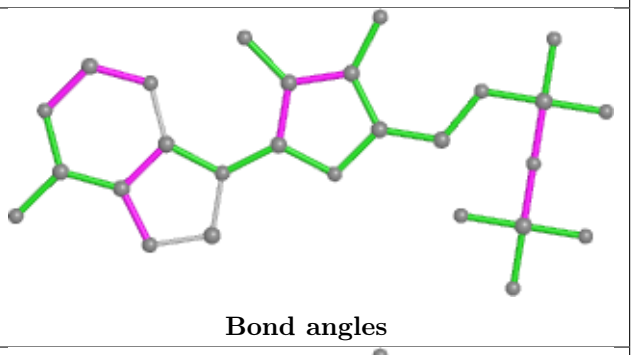


Rings

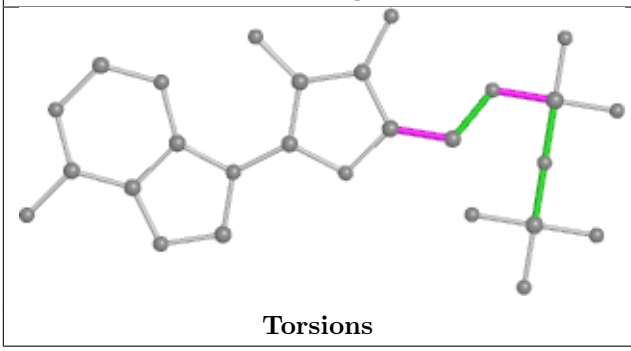
Ligand ADP C 499



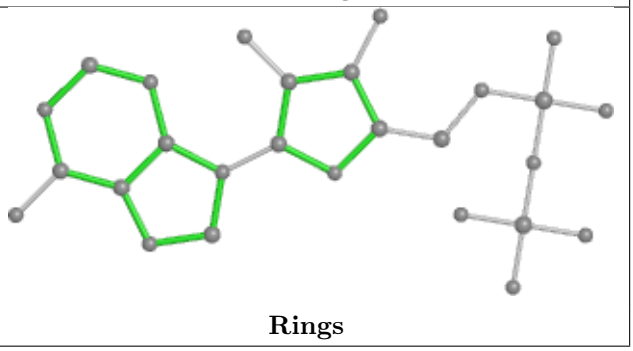
Bond lengths



Bond angles

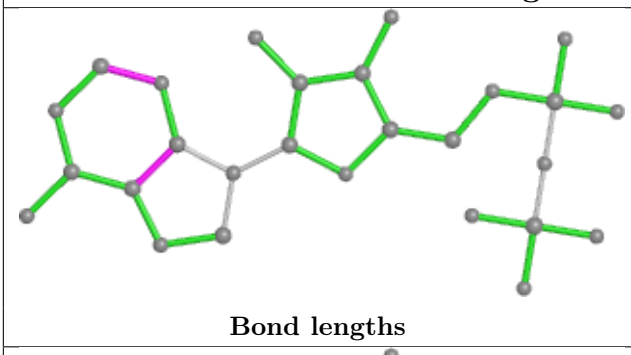


Torsions

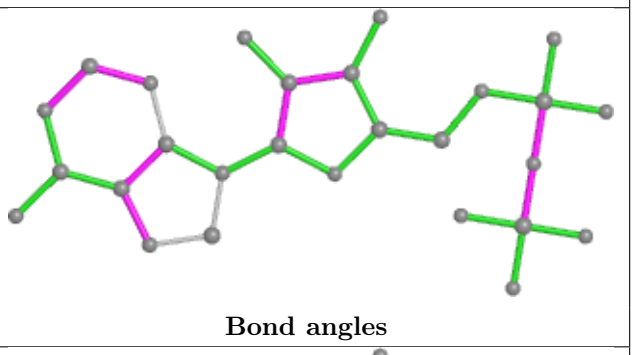


Rings

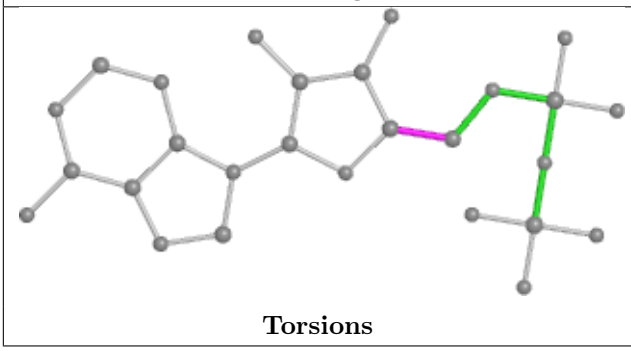
Ligand ADP B 499



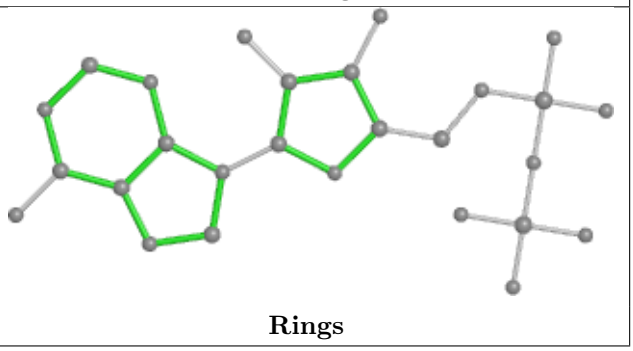
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	488/501 (97%)	0.16	20 (4%)	37	36	27, 41, 49, 56	0
1	B	487/501 (97%)	0.18	24 (4%)	29	28	22, 36, 45, 51	0
1	C	486/501 (97%)	0.18	20 (4%)	37	36	27, 41, 49, 55	0
1	D	486/501 (97%)	0.09	15 (3%)	49	49	21, 36, 45, 51	0
All	All	1947/2004 (97%)	0.15	79 (4%)	37	36	21, 39, 47, 56	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	GLN	4.1
1	B	80	ASN	4.0
1	B	401	ASP	4.0
1	B	116	GLN	3.9
1	B	400	ILE	3.7
1	D	402	VAL	3.3
1	B	244	ASP	3.3
1	D	247	ALA	3.1
1	A	498	GLU	3.1
1	B	119	TYR	3.0
1	B	282	GLU	3.0
1	C	474	ASP	3.0
1	C	400	ILE	3.0
1	C	163	THR	3.0
1	C	399	GLY	2.9
1	D	403	GLN	2.9
1	C	438	THR	2.9
1	C	80	ASN	2.9
1	B	163	THR	2.9
1	B	257	ARG	2.9
1	C	279	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	164	ILE	2.8
1	A	471	PRO	2.8
1	A	152	GLU	2.8
1	D	80	ASN	2.8
1	A	247	ALA	2.7
1	A	402	VAL	2.7
1	D	245	GLN	2.7
1	C	464	LYS	2.6
1	C	277	LYS	2.6
1	B	245	GLN	2.5
1	C	282	GLU	2.5
1	A	187	ARG	2.5
1	A	116	GLN	2.5
1	C	244	ASP	2.5
1	C	82	ARG	2.4
1	A	454	GLU	2.4
1	B	399	GLY	2.4
1	B	84	THR	2.4
1	D	79	THR	2.4
1	D	398	SER	2.4
1	A	183	SER	2.3
1	B	454	GLU	2.3
1	D	244	ASP	2.3
1	D	476	GLY	2.3
1	A	163	THR	2.3
1	A	155	GLU	2.3
1	D	85	THR	2.3
1	A	243	GLY	2.3
1	D	116	GLN	2.3
1	C	278	ALA	2.3
1	B	83	GLU	2.3
1	B	114	LEU	2.2
1	A	472	LYS	2.2
1	D	82	ARG	2.2
1	B	184	ASN	2.1
1	C	245	GLN	2.1
1	B	188	THR	2.1
1	A	428	SER	2.1
1	B	82	ARG	2.1
1	D	243	GLY	2.1
1	A	195	ASP	2.1
1	B	247	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	162	GLY	2.1
1	B	79	THR	2.1
1	A	158	ASP	2.1
1	A	427	THR	2.1
1	B	85	THR	2.1
1	D	84	THR	2.1
1	A	401	ASP	2.1
1	C	401	ASP	2.1
1	A	468	LYS	2.0
1	D	69	ARG	2.0
1	C	79	THR	2.0
1	C	280	LYS	2.0
1	C	184	ASN	2.0
1	C	85	THR	2.0
1	B	205	LEU	2.0
1	C	294	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
2	ADP	C	499	27/27	0.83	0.22	82,95,98,99	0
4	PO4	A	503	5/5	0.89	0.43	44,45,51,51	5
4	PO4	D	503	5/5	0.89	0.35	32,41,42,47	5
2	ADP	B	499	27/27	0.90	0.17	49,62,75,75	0
2	ADP	A	499	27/27	0.91	0.15	53,66,71,72	0
2	ADP	D	499	27/27	0.91	0.14	51,59,69,70	0
4	PO4	C	501	5/5	0.92	0.28	33,37,43,44	5

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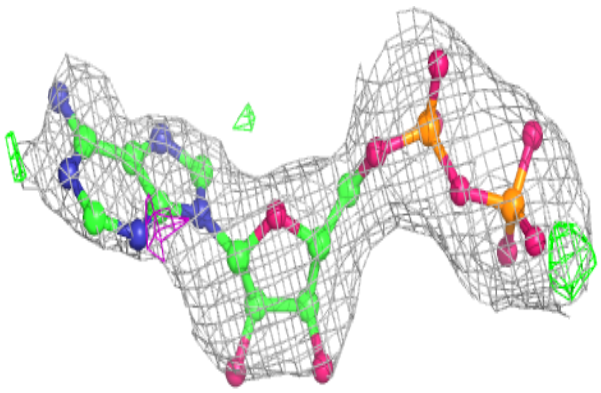
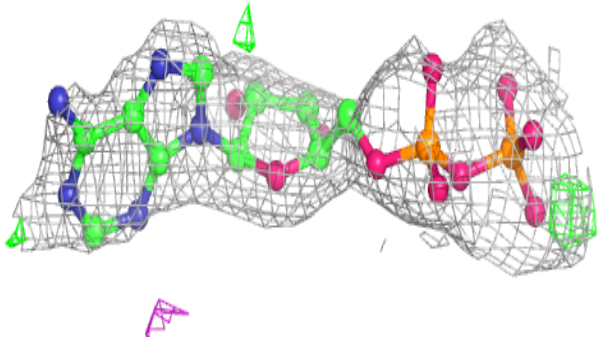
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PO4	A	502	5/5	0.93	0.13	75,79,81,81	0
3	GOL	C	500	6/6	0.94	0.49	57,60,61,63	0
4	PO4	B	501	5/5	0.94	0.36	34,41,47,47	5
3	GOL	D	500	6/6	0.94	0.36	31,31,34,35	0
4	PO4	D	502	5/5	0.94	0.11	71,75,76,79	0
3	GOL	A	500	6/6	0.94	0.30	49,51,53,54	0
5	CL	B	502	1/1	0.94	0.21	76,76,76,76	0
5	CL	C	502	1/1	0.95	0.11	50,50,50,50	0
3	GOL	B	500	6/6	0.96	0.47	41,45,47,48	0
4	PO4	A	501	5/5	0.97	0.07	68,70,75,77	0
5	CL	A	504	1/1	0.97	0.20	69,69,69,69	0
5	CL	D	504	1/1	0.97	0.14	63,63,63,63	0
4	PO4	D	501	5/5	0.98	0.07	81,82,83,85	0

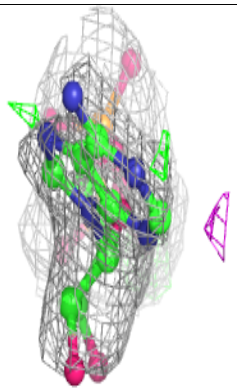
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 499:

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

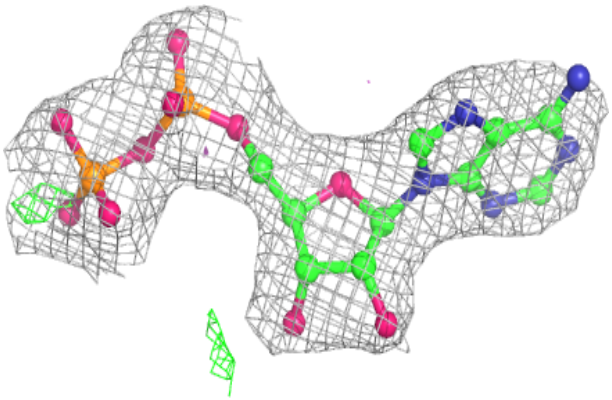


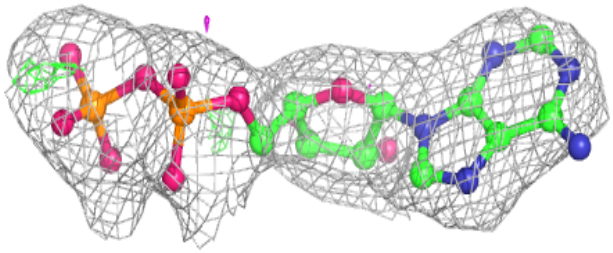


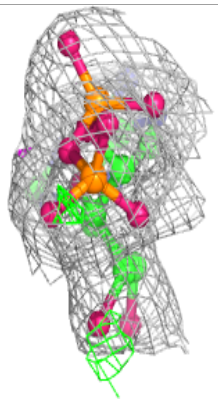


Electron density around ADP B 499:

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

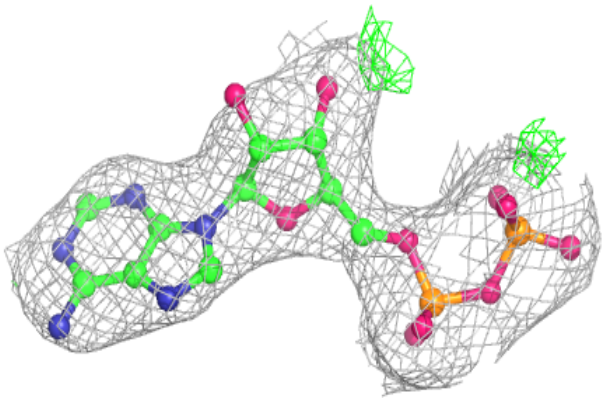


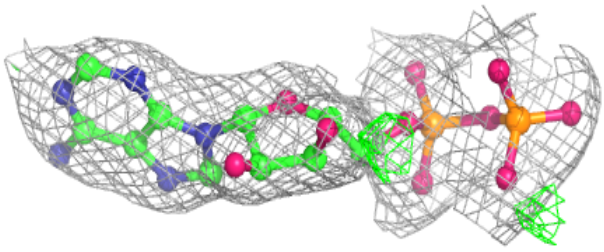


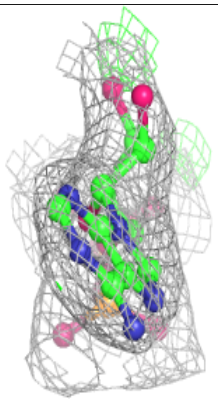


Electron density around ADP A 499:

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

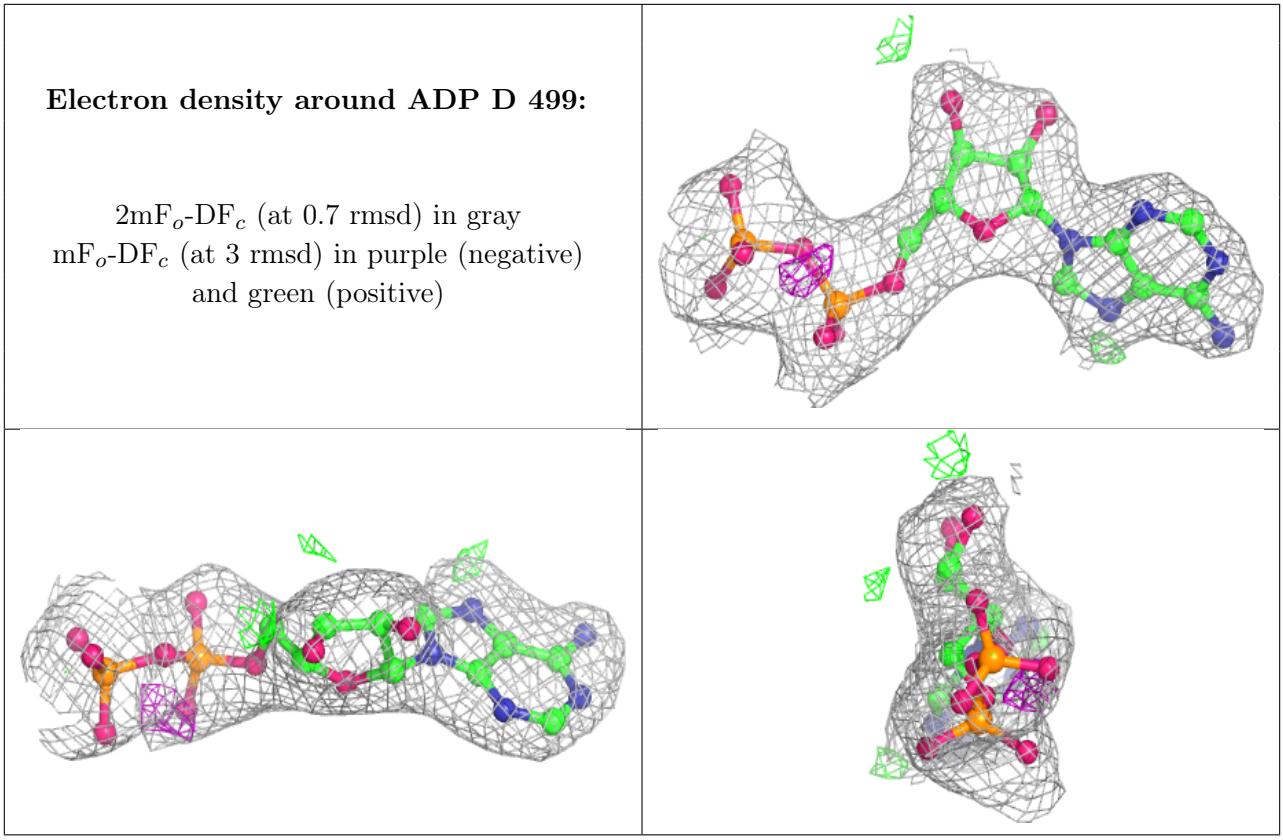






Electron density around ADP D 499:

$2mF_o$-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.