



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:02 am BST

PDB ID : 3QC9
Title : Crystal structure of cross-linked bovine GRK1 T8C/N480C double mutant complexed with ADP and Mg
Authors : Huang, C.-C.; Tesmer, J.J.G.
Deposited on : 2011-01-15
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

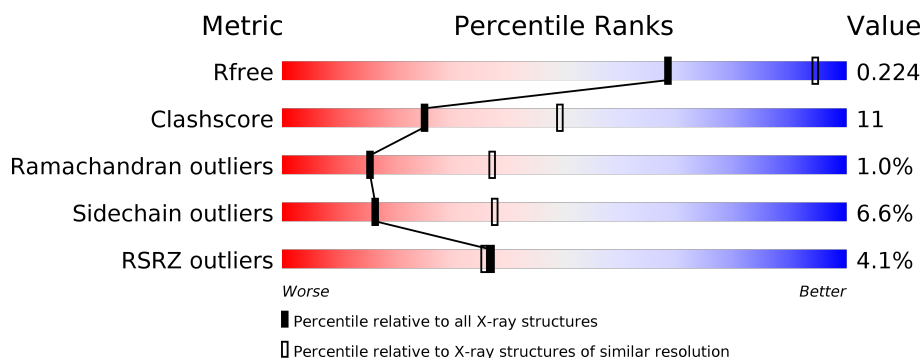
1 Overall quality at a glance ⓘ

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 on 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	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>20%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	543	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	543	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	543	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>22%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15806 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 Rhodopsin kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3904	2507	673	705	19			
1	B	481	Total	C	N	O	S	0	0	0
			3872	2486	667	700	19			
1	C	482	Total	C	N	O	S	0	0	0
			3885	2497	669	700	19			
1	D	486	Total	C	N	O	S	0	0	0
			3904	2507	673	705	19			

There are 40 discrepancies between the modelled and reference sequences:

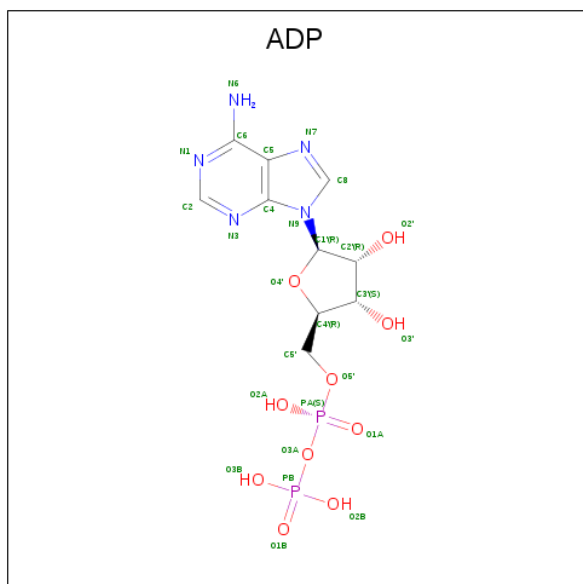
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	CYS	THR	ENGINEERED MUTATION	UNP P28327
A	480	CYS	ASN	ENGINEERED MUTATION	UNP P28327
A	536	VAL	-	EXPRESSION TAG	UNP P28327
A	537	ASP	-	EXPRESSION TAG	UNP P28327
A	538	HIS	-	EXPRESSION TAG	UNP P28327
A	539	HIS	-	EXPRESSION TAG	UNP P28327
A	540	HIS	-	EXPRESSION TAG	UNP P28327
A	541	HIS	-	EXPRESSION TAG	UNP P28327
A	542	HIS	-	EXPRESSION TAG	UNP P28327
A	543	HIS	-	EXPRESSION TAG	UNP P28327
B	8	CYS	THR	ENGINEERED MUTATION	UNP P28327
B	480	CYS	ASN	ENGINEERED MUTATION	UNP P28327
B	536	VAL	-	EXPRESSION TAG	UNP P28327
B	537	ASP	-	EXPRESSION TAG	UNP P28327
B	538	HIS	-	EXPRESSION TAG	UNP P28327
B	539	HIS	-	EXPRESSION TAG	UNP P28327
B	540	HIS	-	EXPRESSION TAG	UNP P28327
B	541	HIS	-	EXPRESSION TAG	UNP P28327
B	542	HIS	-	EXPRESSION TAG	UNP P28327
B	543	HIS	-	EXPRESSION TAG	UNP P28327
C	8	CYS	THR	ENGINEERED MUTATION	UNP P28327

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Chain	Residue	Modelled	Actual	Comment	Reference
C	480	CYS	ASN	ENGINEERED MUTATION	UNP P28327
C	536	VAL	-	EXPRESSION TAG	UNP P28327
C	537	ASP	-	EXPRESSION TAG	UNP P28327
C	538	HIS	-	EXPRESSION TAG	UNP P28327
C	539	HIS	-	EXPRESSION TAG	UNP P28327
C	540	HIS	-	EXPRESSION TAG	UNP P28327
C	541	HIS	-	EXPRESSION TAG	UNP P28327
C	542	HIS	-	EXPRESSION TAG	UNP P28327
C	543	HIS	-	EXPRESSION TAG	UNP P28327
D	8	CYS	THR	ENGINEERED MUTATION	UNP P28327
D	480	CYS	ASN	ENGINEERED MUTATION	UNP P28327
D	536	VAL	-	EXPRESSION TAG	UNP P28327
D	537	ASP	-	EXPRESSION TAG	UNP P28327
D	538	HIS	-	EXPRESSION TAG	UNP P28327
D	539	HIS	-	EXPRESSION TAG	UNP P28327
D	540	HIS	-	EXPRESSION TAG	UNP P28327
D	541	HIS	-	EXPRESSION TAG	UNP P28327
D	542	HIS	-	EXPRESSION TAG	UNP P28327
D	543	HIS	-	EXPRESSION TAG	UNP P28327

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



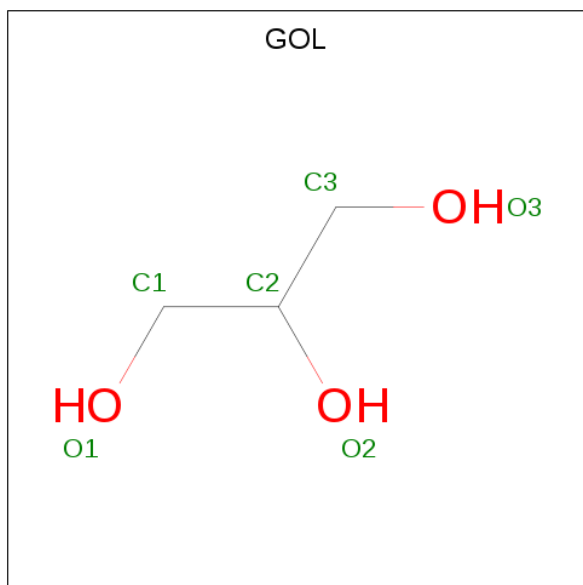
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

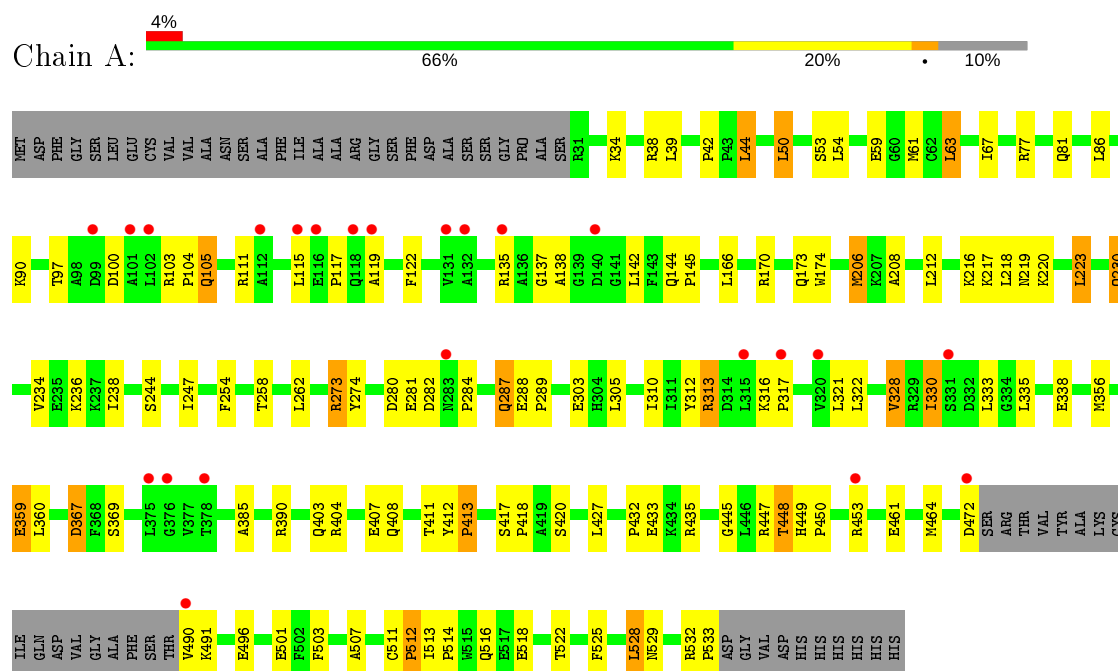
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total 30	O 30	0	0
5	B	32	Total 32	O 32	0	0
5	C	26	Total 26	O 26	0	0
5	D	25	Total 25	O 25	0	0

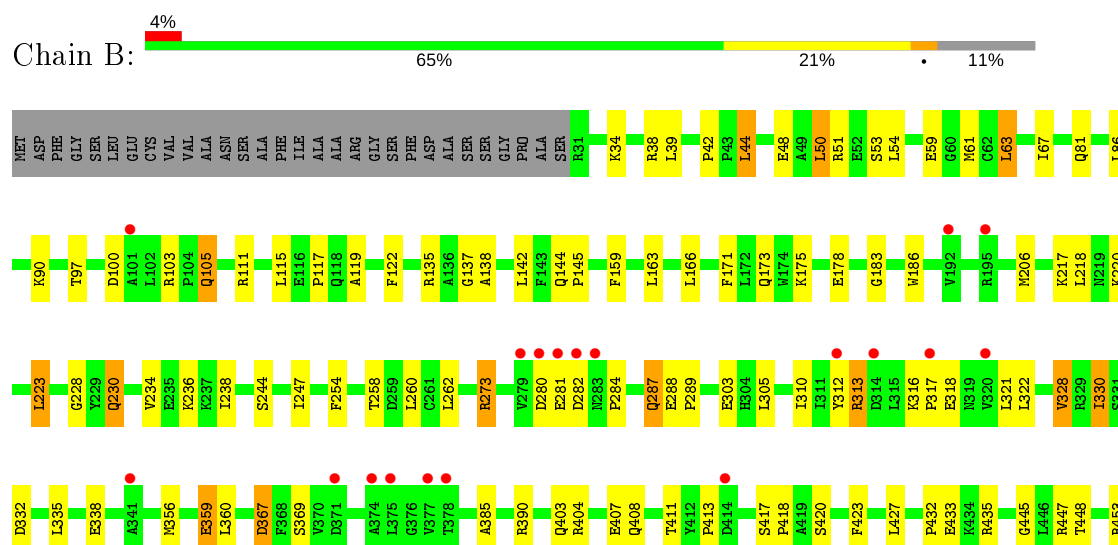
3 Residue-property plots [i](#)

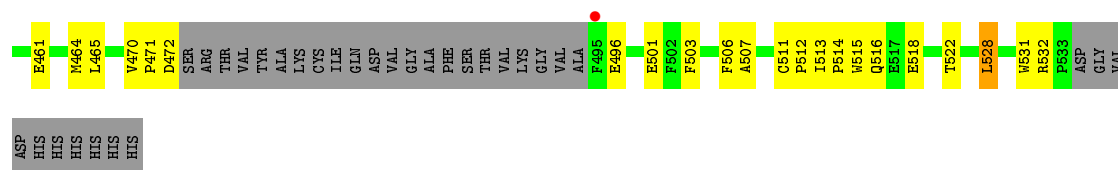
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Rhodopsin kinase

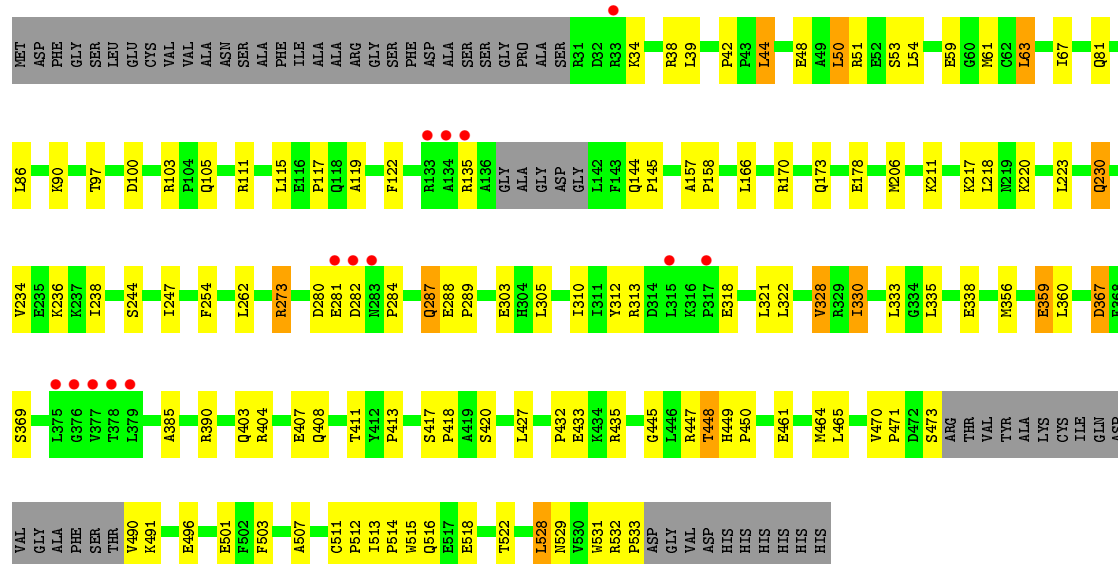


• Molecule 1: Rhodopsin kinase

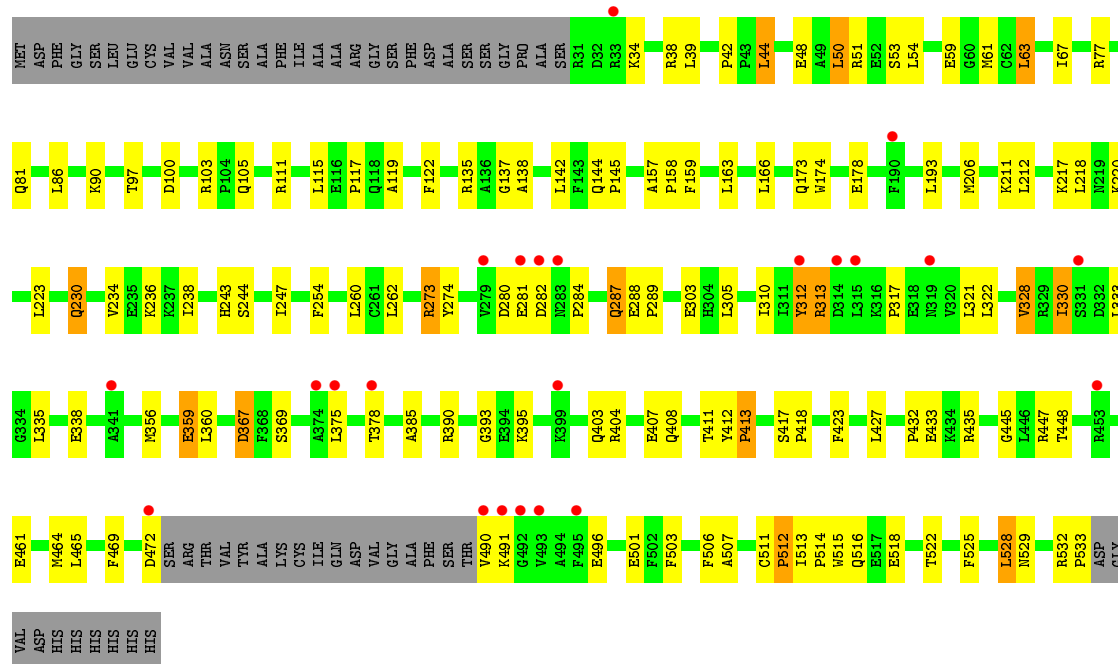




• Molecule 1: Rhodopsin kinase



• Molecule 1: Rhodopsin kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.70Å 89.97Å 122.64Å 88.07° 90.26° 68.78°	Depositor
Resolution (Å)	29.60 – 2.70 29.60 – 2.68	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.60-2.70) 88.1 (29.60-2.68)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.192 , 0.229 0.187 , 0.224	Depositor DCC
R_{free} test set	3089 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.125 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15806	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: GOL, MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/3997	0.56	0/5391
1	B	0.43	0/3965	0.56	0/5348
1	C	0.42	0/3977	0.56	0/5363
1	D	0.43	0/3997	0.56	0/5391
All	All	0.43	0/15936	0.56	0/21493

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3904	0	3874	84	0
1	B	3872	0	3835	89	0
1	C	3885	0	3860	77	0
1	D	3904	0	3874	92	0
2	A	27	0	12	3	0
2	B	27	0	12	3	0
2	C	27	0	12	1	0
2	D	27	0	12	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0
5	A	30	0	0	3	0
5	B	32	0	0	4	0
5	C	26	0	0	3	0
5	D	25	0	0	2	0
All	All	15806	0	15507	334	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (334) 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:D:359:GLU:HG2	1:D:432:PRO:HG3	1.42	0.98
1:A:359:GLU:HG2	1:A:432:PRO:HG3	1.48	0.94
1:B:359:GLU:HG2	1:B:432:PRO:HG3	1.46	0.94
1:C:359:GLU:HG2	1:C:432:PRO:HG3	1.49	0.93
1:B:166:LEU:HD23	1:C:44:LEU:HD21	1.56	0.87
1:D:238:ILE:HD12	1:D:310:ILE:HD13	1.56	0.87
1:C:238:ILE:HD12	1:C:310:ILE:HD13	1.58	0.85
1:B:322:LEU:HD23	1:B:328:VAL:HG23	1.57	0.85
1:B:238:ILE:HD12	1:B:310:ILE:HD13	1.60	0.83
1:A:322:LEU:HD23	1:A:328:VAL:HG23	1.59	0.83
1:C:322:LEU:HD23	1:C:328:VAL:HG23	1.61	0.82
1:B:111:ARG:HA	1:B:115:LEU:HD12	1.62	0.82
1:A:111:ARG:HA	1:A:115:LEU:HD12	1.61	0.80
1:D:111:ARG:HA	1:D:115:LEU:HD12	1.63	0.80
1:A:238:ILE:HD12	1:A:310:ILE:HD13	1.62	0.80
1:C:111:ARG:HA	1:C:115:LEU:HD12	1.64	0.80
1:D:322:LEU:HD23	1:D:328:VAL:HG23	1.63	0.78
1:A:518:GLU:O	1:A:522:THR:HG22	1.86	0.74
1:B:234:VAL:O	1:B:238:ILE:HG12	1.87	0.74
1:D:518:GLU:O	1:D:522:THR:HG22	1.87	0.74
1:D:34:LYS:HE2	1:D:38:ARG:HH21	1.53	0.73
1:C:322:LEU:CD2	1:C:328:VAL:HG23	2.17	0.73
1:B:34:LYS:HE2	1:B:38:ARG:HH21	1.53	0.73
1:D:234:VAL:O	1:D:238:ILE:HG12	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:O	1:A:238:ILE:HG12	1.88	0.73
1:D:511:CYS:O	1:D:514:PRO:HD2	1.90	0.72
1:B:511:CYS:O	1:B:514:PRO:HD2	1.90	0.72
1:C:234:VAL:O	1:C:238:ILE:HG12	1.90	0.72
1:A:322:LEU:CD2	1:A:328:VAL:HG23	2.19	0.71
1:B:322:LEU:CD2	1:B:328:VAL:HG23	2.20	0.71
1:D:367:ASP:HB3	1:D:369:SER:H	1.55	0.71
1:C:367:ASP:HB3	1:C:369:SER:H	1.56	0.71
1:C:518:GLU:O	1:C:522:THR:HG22	1.91	0.71
1:C:34:LYS:HE2	1:C:38:ARG:HH21	1.54	0.71
1:B:44:LEU:HD21	1:C:166:LEU:HD23	1.72	0.70
1:B:518:GLU:O	1:B:522:THR:HG22	1.91	0.70
1:C:511:CYS:O	1:C:514:PRO:HD2	1.92	0.69
1:A:511:CYS:O	1:A:514:PRO:HD2	1.91	0.69
1:A:34:LYS:HE2	1:A:38:ARG:HH21	1.57	0.69
1:D:39:LEU:O	1:D:528:LEU:HD11	1.93	0.69
1:B:39:LEU:O	1:B:528:LEU:HD11	1.92	0.69
1:A:44:LEU:HD21	1:D:166:LEU:HD23	1.75	0.69
1:D:322:LEU:CD2	1:D:328:VAL:HG23	2.23	0.68
1:B:111:ARG:HH22	1:B:137:GLY:HA3	1.58	0.67
1:D:111:ARG:HH22	1:D:137:GLY:HA3	1.60	0.67
1:B:367:ASP:HB3	1:B:369:SER:H	1.58	0.67
1:A:367:ASP:HB3	1:A:369:SER:H	1.59	0.67
1:A:39:LEU:O	1:A:528:LEU:HD11	1.95	0.66
2:A:700:ADP:O2B	5:A:548:HOH:O	2.12	0.66
1:C:39:LEU:O	1:C:528:LEU:HD11	1.95	0.66
1:A:97:THR:HG22	1:A:97:THR:O	1.96	0.65
1:A:166:LEU:HD23	1:D:44:LEU:HD21	1.79	0.65
1:A:453:ARG:HH12	1:B:105:GLN:HB3	1.62	0.64
1:A:111:ARG:HH22	1:A:137:GLY:HA3	1.62	0.64
1:A:59:GLU:HA	1:A:63:LEU:HD22	1.81	0.63
1:B:59:GLU:HA	1:B:63:LEU:HD22	1.81	0.63
1:A:490:VAL:HG22	1:A:491:LYS:H	1.65	0.62
2:B:700:ADP:H5'2	5:B:545:HOH:O	1.99	0.62
2:D:700:ADP:H5'2	5:D:544:HOH:O	1.99	0.62
1:D:59:GLU:HA	1:D:63:LEU:HD22	1.80	0.61
1:A:220:LYS:HE2	1:A:503:PHE:CD1	2.35	0.61
1:B:230:GLN:O	1:B:234:VAL:HG23	2.00	0.61
1:B:42:PRO:HD2	1:B:173:GLN:HB3	1.82	0.61
1:C:490:VAL:HG22	1:C:491:LYS:H	1.64	0.60
1:A:105:GLN:HB3	1:B:453:ARG:HH12	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLU:HA	1:C:63:LEU:HD22	1.82	0.60
1:D:490:VAL:HG22	1:D:491:LYS:H	1.66	0.60
1:D:305:LEU:HD11	1:D:330:ILE:HD11	1.83	0.60
1:D:97:THR:O	1:D:97:THR:HG22	2.01	0.60
1:B:217:LYS:O	1:B:218:LEU:HD23	2.02	0.60
1:C:42:PRO:HD2	1:C:173:GLN:HB3	1.83	0.59
1:C:513:ILE:HD13	5:C:559:HOH:O	2.02	0.59
1:D:230:GLN:O	1:D:234:VAL:HG23	2.01	0.59
1:C:220:LYS:HE2	1:C:503:PHE:CD1	2.38	0.59
1:D:50:LEU:HD23	1:D:50:LEU:C	2.23	0.59
1:D:117:PRO:HA	1:D:122:PHE:CD1	2.38	0.59
1:C:97:THR:O	1:C:97:THR:HG22	2.03	0.59
2:A:700:ADP:PB	5:A:548:HOH:O	2.59	0.58
1:D:220:LYS:HE2	1:D:503:PHE:CD1	2.38	0.58
1:B:220:LYS:HE2	1:B:503:PHE:CD1	2.39	0.58
1:B:230:GLN:HG2	5:B:565:HOH:O	2.03	0.58
1:D:303:GLU:CD	1:D:447:ARG:HH21	2.07	0.57
1:A:42:PRO:HD2	1:A:173:GLN:HB3	1.87	0.57
1:C:230:GLN:O	1:C:234:VAL:HG23	2.03	0.57
1:C:50:LEU:C	1:C:50:LEU:HD23	2.24	0.57
1:A:50:LEU:HD23	1:A:50:LEU:C	2.25	0.57
1:A:230:GLN:O	1:A:234:VAL:HG23	2.05	0.57
1:B:303:GLU:CD	1:B:447:ARG:HH21	2.07	0.57
1:D:42:PRO:HD2	1:D:173:GLN:HB3	1.87	0.57
1:B:117:PRO:HA	1:B:122:PHE:CD1	2.40	0.57
1:B:50:LEU:HD23	1:B:50:LEU:C	2.27	0.55
1:A:117:PRO:HA	1:A:122:PHE:CD1	2.40	0.55
1:D:404:ARG:O	1:D:408:GLN:HB3	2.07	0.55
1:A:303:GLU:CD	1:A:447:ARG:HH21	2.10	0.55
1:A:67:ILE:HG13	1:A:516:GLN:HB3	1.87	0.55
1:B:305:LEU:HD11	1:B:330:ILE:HD11	1.89	0.55
1:B:97:THR:O	1:B:97:THR:HG22	2.06	0.54
1:D:50:LEU:O	1:D:54:LEU:HG	2.08	0.54
1:C:513:ILE:HB	1:C:514:PRO:HD3	1.90	0.54
1:A:97:THR:CG2	1:A:97:THR:O	2.55	0.53
1:A:404:ARG:O	1:A:408:GLN:HB3	2.09	0.53
1:C:403:GLN:O	1:C:407:GLU:HG2	2.09	0.53
1:B:321:LEU:O	1:B:328:VAL:HA	2.09	0.53
1:C:117:PRO:HA	1:C:122:PHE:CD1	2.44	0.53
1:D:178:GLU:HB2	1:D:515:TRP:CZ3	2.44	0.53
1:D:67:ILE:HG13	1:D:516:GLN:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:LEU:HD11	1:C:330:ILE:HD11	1.91	0.53
1:B:111:ARG:NH2	1:B:137:GLY:HA3	2.23	0.52
1:D:97:THR:CG2	1:D:97:THR:O	2.57	0.52
1:C:404:ARG:O	1:C:408:GLN:HB3	2.09	0.52
1:A:533:PRO:HG2	1:D:77:ARG:HG3	1.90	0.52
1:A:445:GLY:O	1:A:448:THR:HB	2.10	0.52
1:C:303:GLU:CD	1:C:447:ARG:HH21	2.12	0.52
1:A:100:ASP:HA	1:A:103:ARG:HG3	1.92	0.51
1:A:97:THR:HG23	1:A:464:MET:HE1	1.92	0.51
1:D:403:GLN:O	1:D:407:GLU:HG2	2.10	0.51
1:B:359:GLU:CG	1:B:432:PRO:HG3	2.31	0.51
1:D:445:GLY:O	1:D:448:THR:HB	2.10	0.51
1:C:313:ARG:HD3	1:C:335:LEU:O	2.10	0.51
1:B:50:LEU:O	1:B:54:LEU:HG	2.10	0.51
1:B:97:THR:HG23	1:B:464:MET:HE1	1.92	0.51
1:B:178:GLU:HB2	1:B:515:TRP:CZ3	2.45	0.51
1:B:86:LEU:HD11	1:B:90:LYS:HE3	1.92	0.51
1:C:50:LEU:O	1:C:54:LEU:HG	2.11	0.51
1:A:313:ARG:HD3	1:A:335:LEU:O	2.11	0.50
1:A:321:LEU:O	1:A:328:VAL:HA	2.10	0.50
1:B:403:GLN:O	1:B:407:GLU:HG2	2.10	0.50
1:D:321:LEU:O	1:D:328:VAL:HA	2.11	0.50
1:A:77:ARG:HG3	1:D:533:PRO:HG2	1.93	0.50
1:B:282:ASP:C	1:B:284:PRO:HD3	2.32	0.50
1:B:67:ILE:HG13	1:B:516:GLN:HB3	1.93	0.50
1:C:97:THR:CG2	1:C:97:THR:O	2.59	0.50
1:C:528:LEU:HD23	1:C:528:LEU:N	2.27	0.50
1:A:403:GLN:O	1:A:407:GLU:HG2	2.12	0.50
1:C:97:THR:HG23	1:C:464:MET:HE1	1.92	0.50
1:D:111:ARG:NH2	1:D:137:GLY:HA3	2.25	0.50
1:D:359:GLU:CG	1:D:432:PRO:HG3	2.28	0.50
1:C:321:LEU:O	1:C:328:VAL:HA	2.11	0.50
1:A:282:ASP:C	1:A:284:PRO:HD3	2.32	0.49
1:B:404:ARG:O	1:B:408:GLN:HB3	2.11	0.49
1:B:50:LEU:HA	1:B:53:SER:OG	2.11	0.49
1:A:453:ARG:HH12	1:B:105:GLN:CB	2.25	0.49
1:D:313:ARG:HD3	1:D:335:LEU:O	2.12	0.49
1:D:518:GLU:O	1:D:522:THR:CG2	2.59	0.49
1:A:305:LEU:HD11	1:A:330:ILE:HD11	1.93	0.49
1:A:111:ARG:NH2	1:A:137:GLY:HA3	2.26	0.49
1:A:528:LEU:N	1:A:528:LEU:HD23	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLY:O	1:B:448:THR:HB	2.13	0.49
1:C:445:GLY:O	1:C:448:THR:HB	2.13	0.49
2:A:700:ADP:H5'	5:A:545:HOH:O	2.11	0.49
1:D:50:LEU:HA	1:D:53:SER:OG	2.12	0.49
1:B:513:ILE:HB	1:B:514:PRO:HD3	1.95	0.49
1:C:67:ILE:HG13	1:C:516:GLN:HB3	1.94	0.49
2:C:700:ADP:PB	5:C:547:HOH:O	2.71	0.49
1:A:137:GLY:HA2	1:A:142:LEU:HD11	1.94	0.48
1:A:513:ILE:HB	1:A:514:PRO:HD3	1.94	0.48
1:B:137:GLY:HA2	1:B:142:LEU:HD11	1.94	0.48
1:D:217:LYS:O	1:D:218:LEU:HD23	2.13	0.48
1:A:217:LYS:O	1:A:218:LEU:HD23	2.13	0.48
1:A:50:LEU:HA	1:A:53:SER:OG	2.14	0.48
1:B:417:SER:O	1:B:418:PRO:C	2.51	0.48
1:A:86:LEU:HD11	1:A:90:LYS:HE3	1.94	0.48
1:D:193:LEU:HD13	2:D:700:ADP:C2	2.49	0.48
1:B:273:ARG:HB3	1:B:317:PRO:HB2	1.95	0.48
1:B:531:TRP:HB2	1:C:531:TRP:CG	2.48	0.48
1:D:513:ILE:HB	1:D:514:PRO:HD3	1.95	0.48
1:A:219:ASN:HD22	4:A:544:GOL:H2	1.79	0.48
1:C:282:ASP:C	1:C:284:PRO:HD3	2.34	0.48
1:B:313:ARG:HD3	1:B:335:LEU:O	2.14	0.47
1:C:217:LYS:O	1:C:218:LEU:HD23	2.14	0.47
1:C:449:HIS:CG	1:C:450:PRO:HD2	2.49	0.47
1:D:282:ASP:C	1:D:284:PRO:HD3	2.34	0.47
1:A:50:LEU:O	1:A:54:LEU:HG	2.15	0.47
1:A:322:LEU:HD23	1:A:328:VAL:CG2	2.39	0.47
1:B:236:LYS:HG3	1:B:262:LEU:HD21	1.96	0.47
1:A:236:LYS:HG3	1:A:262:LEU:HD21	1.95	0.47
1:D:97:THR:HG23	1:D:464:MET:HE1	1.96	0.47
1:C:312:TYR:O	1:C:313:ARG:HB2	2.15	0.47
1:A:312:TYR:O	1:A:313:ARG:HB2	2.14	0.47
2:B:700:ADP:O5'	2:B:700:ADP:H8	1.98	0.47
1:C:144:GLN:N	1:C:145:PRO:HD2	2.30	0.47
1:B:254:PHE:HA	1:B:507:ALA:HB1	1.97	0.46
1:C:490:VAL:HG22	1:C:491:LYS:N	2.30	0.46
1:C:86:LEU:HD11	1:C:90:LYS:HE3	1.97	0.46
1:A:254:PHE:HA	1:A:507:ALA:HB1	1.97	0.46
1:B:159:PHE:CZ	1:B:163:LEU:HD21	2.49	0.46
1:B:423:PHE:CE2	1:B:427:LEU:HD11	2.50	0.46
1:C:50:LEU:HA	1:C:53:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:LYS:HG3	1:D:262:LEU:HD21	1.98	0.46
1:B:97:THR:O	1:B:97:THR:CG2	2.63	0.46
1:A:356:MET:HB3	1:A:360:LEU:HD22	1.96	0.46
1:D:287:GLN:HE21	1:D:287:GLN:HA	1.81	0.46
1:C:322:LEU:HD23	1:C:328:VAL:CG2	2.39	0.46
1:D:144:GLN:N	1:D:145:PRO:HD2	2.30	0.46
1:A:287:GLN:HE21	1:A:287:GLN:HA	1.80	0.46
1:C:496:GLU:OE1	1:C:496:GLU:HA	2.16	0.46
1:D:86:LEU:HD11	1:D:90:LYS:HE3	1.97	0.46
1:C:287:GLN:HA	1:C:287:GLN:HE21	1.79	0.46
1:D:34:LYS:CE	1:D:38:ARG:HH21	2.27	0.46
1:D:137:GLY:HA2	1:D:142:LEU:HD11	1.97	0.46
1:D:211:LYS:HD3	1:D:518:GLU:HG3	1.97	0.46
1:D:356:MET:HB3	1:D:360:LEU:HD22	1.98	0.46
1:B:287:GLN:HA	1:B:287:GLN:HE21	1.80	0.46
1:C:417:SER:O	1:C:418:PRO:C	2.54	0.46
1:C:288:GLU:CD	1:C:420:SER:HG	2.20	0.46
1:D:412:TYR:HA	1:D:413:PRO:HD2	1.85	0.45
1:B:531:TRP:CB	1:C:531:TRP:CB	2.94	0.45
1:B:260:LEU:HB3	1:B:506:PHE:CE2	2.51	0.45
1:B:228:GLY:HA2	5:B:565:HOH:O	2.16	0.45
1:C:254:PHE:HA	1:C:507:ALA:HB1	1.98	0.45
1:D:254:PHE:HA	1:D:507:ALA:HB1	1.98	0.45
1:D:423:PHE:CE2	1:D:427:LEU:HD11	2.51	0.45
1:A:273:ARG:HG3	1:A:274:TYR:N	2.31	0.45
1:A:238:ILE:HG21	1:A:333:LEU:HD22	1.98	0.45
1:B:111:ARG:NH2	1:B:137:GLY:CA	2.80	0.45
1:B:427:LEU:O	1:B:435:ARG:HD3	2.17	0.45
1:D:159:PHE:CZ	1:D:163:LEU:HD21	2.52	0.45
1:D:427:LEU:O	1:D:435:ARG:HD3	2.17	0.45
1:B:312:TYR:O	1:B:313:ARG:HB2	2.16	0.44
1:A:312:TYR:CE2	1:A:330:ILE:HD12	2.52	0.44
1:D:312:TYR:O	1:D:313:ARG:HB2	2.17	0.44
1:A:518:GLU:O	1:A:522:THR:CG2	2.60	0.44
1:B:100:ASP:HA	1:B:103:ARG:HG3	1.98	0.44
1:B:518:GLU:O	1:B:522:THR:CG2	2.63	0.44
1:A:137:GLY:HA2	1:A:142:LEU:CD1	2.48	0.44
1:C:288:GLU:HB2	1:C:289:PRO:HD3	2.00	0.44
1:C:238:ILE:HG21	1:C:333:LEU:HD22	1.99	0.44
1:B:531:TRP:CG	1:C:531:TRP:HB2	2.53	0.44
1:D:465:LEU:HA	1:D:465:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLN:N	1:B:145:PRO:HD2	2.33	0.44
1:C:100:ASP:HA	1:C:103:ARG:HG3	1.99	0.44
1:C:157:ALA:N	1:C:158:PRO:CD	2.80	0.44
1:A:490:VAL:HG22	1:A:491:LYS:N	2.30	0.44
1:C:356:MET:HB3	1:C:360:LEU:HD22	2.00	0.44
1:C:359:GLU:CG	1:C:432:PRO:HG3	2.33	0.44
1:D:244:SER:HB3	1:D:247:ILE:HG12	1.99	0.44
1:B:322:LEU:HD23	1:B:328:VAL:CG2	2.38	0.44
1:D:288:GLU:HB2	1:D:289:PRO:HD3	1.99	0.44
1:A:144:GLN:N	1:A:145:PRO:HD2	2.32	0.43
1:A:244:SER:HB3	1:A:247:ILE:HG12	2.00	0.43
1:A:359:GLU:CG	1:A:432:PRO:HG3	2.33	0.43
1:D:157:ALA:N	1:D:158:PRO:CD	2.81	0.43
1:A:449:HIS:CG	1:A:450:PRO:HD2	2.53	0.43
1:C:427:LEU:O	1:C:435:ARG:HD3	2.18	0.43
1:C:513:ILE:CD1	5:C:559:HOH:O	2.61	0.43
1:B:217:LYS:C	1:B:218:LEU:HD23	2.38	0.43
1:D:211:LYS:CD	1:D:518:GLU:HG3	2.48	0.43
1:B:284:PRO:HB2	1:B:385:ALA:CB	2.48	0.43
1:A:496:GLU:OE1	1:A:496:GLU:HA	2.19	0.43
1:B:244:SER:HB3	1:B:247:ILE:HG12	2.01	0.43
1:A:417:SER:O	1:A:418:PRO:C	2.57	0.43
1:A:288:GLU:CD	1:A:420:SER:HG	2.22	0.43
1:B:288:GLU:HB2	1:B:289:PRO:HD3	2.00	0.43
1:B:137:GLY:HA2	1:B:142:LEU:CD1	2.49	0.43
1:B:470:VAL:HA	1:B:471:PRO:HD3	1.87	0.43
1:C:244:SER:HB3	1:C:247:ILE:HG12	1.99	0.43
1:C:287:GLN:CA	1:C:287:GLN:HE21	2.32	0.43
1:D:97:THR:HA	1:D:464:MET:HE1	2.01	0.43
1:D:212:LEU:HD23	1:D:212:LEU:HA	1.71	0.42
1:D:393:GLY:O	1:D:395:LYS:HG2	2.19	0.42
1:B:238:ILE:HD11	1:B:338:GLU:HG2	2.00	0.42
1:B:356:MET:HB3	1:B:360:LEU:HD22	2.00	0.42
1:C:465:LEU:HA	1:C:465:LEU:HD23	1.91	0.42
1:C:211:LYS:CD	1:C:518:GLU:HG3	2.49	0.42
1:C:449:HIS:HA	1:C:450:PRO:HD3	1.87	0.42
1:B:496:GLU:OE1	1:B:496:GLU:HA	2.20	0.42
1:D:322:LEU:HD23	1:D:328:VAL:CG2	2.42	0.42
1:D:417:SER:O	1:D:418:PRO:C	2.58	0.42
1:D:48:GLU:O	1:D:51:ARG:HB3	2.20	0.42
1:D:496:GLU:HA	1:D:496:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:PRO:O	1:D:516:GLN:HG3	2.20	0.42
1:C:178:GLU:HB2	1:C:515:TRP:CZ3	2.55	0.42
1:A:316:LYS:HB2	1:A:317:PRO:HD2	2.02	0.42
1:A:532:ARG:NH2	1:D:529:ASN:HB3	2.35	0.42
1:B:48:GLU:O	1:B:51:ARG:HB3	2.20	0.42
1:C:236:LYS:HG3	1:C:262:LEU:HD21	2.00	0.42
1:D:238:ILE:CD1	1:D:310:ILE:HD13	2.38	0.42
1:D:260:LEU:HB3	1:D:506:PHE:CE2	2.55	0.42
1:A:512:PRO:O	1:A:516:GLN:HG3	2.20	0.42
1:B:223:LEU:HA	1:B:223:LEU:HD23	1.87	0.42
1:C:238:ILE:HD11	1:C:338:GLU:HG2	2.02	0.42
1:C:284:PRO:HB2	1:C:385:ALA:CB	2.49	0.42
1:D:238:ILE:HG21	1:D:333:LEU:HD22	2.02	0.42
1:A:284:PRO:HB2	1:A:385:ALA:CB	2.50	0.41
1:A:174:TRP:CZ2	1:A:525:PHE:CD1	3.07	0.41
1:B:273:ARG:HG2	1:B:318:GLU:HB3	2.02	0.41
1:C:144:GLN:N	1:C:145:PRO:CD	2.83	0.41
1:D:243:HIS:HB3	5:D:566:HOH:O	2.20	0.41
1:B:34:LYS:CE	1:B:38:ARG:HH21	2.27	0.41
1:D:238:ILE:HD11	1:D:338:GLU:HG2	2.02	0.41
1:D:273:ARG:HB3	1:D:317:PRO:HB2	2.02	0.41
1:A:111:ARG:NH2	1:A:137:GLY:CA	2.84	0.41
1:A:287:GLN:HE21	1:A:287:GLN:CA	2.33	0.41
1:A:427:LEU:O	1:A:435:ARG:HD3	2.19	0.41
1:B:528:LEU:N	1:B:528:LEU:HD23	2.34	0.41
1:B:59:GLU:HG2	5:B:573:HOH:O	2.20	0.41
1:D:490:VAL:HG22	1:D:491:LYS:N	2.33	0.41
1:B:316:LYS:HB2	1:B:317:PRO:HD2	2.02	0.41
1:B:332:ASP:OD2	2:B:700:ADP:O2A	2.39	0.41
1:D:100:ASP:HA	1:D:103:ARG:HG3	2.03	0.41
1:D:287:GLN:CA	1:D:287:GLN:HE21	2.34	0.41
1:A:216:LYS:HE2	1:A:218:LEU:HD21	2.03	0.41
1:A:238:ILE:HD11	1:A:338:GLU:HG2	2.02	0.41
1:D:528:LEU:N	1:D:528:LEU:HD23	2.36	0.41
1:C:312:TYR:CE2	1:C:330:ILE:HD12	2.56	0.41
1:C:330:ILE:HG21	1:C:330:ILE:HD13	1.79	0.41
1:D:111:ARG:NH2	1:D:137:GLY:CA	2.83	0.41
1:D:144:GLN:N	1:D:145:PRO:CD	2.84	0.41
1:C:470:VAL:HA	1:C:471:PRO:HD3	1.85	0.41
1:D:469:PHE:CD2	1:D:469:PHE:C	2.94	0.41
1:A:206:MET:SD	1:A:208:ALA:HB3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HA	1:A:212:LEU:HD23	1.77	0.41
1:B:532:ARG:HH22	1:C:529:ASN:HB3	1.86	0.41
1:A:529:ASN:HB3	1:D:532:ARG:HH22	1.86	0.41
1:D:284:PRO:HB2	1:D:385:ALA:CB	2.50	0.41
1:D:174:TRP:CZ2	1:D:525:PHE:CD1	3.09	0.41
1:B:465:LEU:HD23	1:B:465:LEU:HA	1.88	0.40
1:A:223:LEU:HA	1:A:223:LEU:HD23	1.82	0.40
1:A:412:TYR:HA	1:A:413:PRO:HD2	1.87	0.40
1:C:273:ARG:HG2	1:C:318:GLU:HB3	2.03	0.40
1:B:183:GLY:O	1:B:186:TRP:HB2	2.21	0.40
1:D:273:ARG:HG3	1:D:274:TYR:N	2.37	0.40
1:D:375:LEU:O	1:D:378:THR:HB	2.21	0.40
1:B:238:ILE:HG23	1:B:310:ILE:HD13	2.04	0.40
1:C:48:GLU:O	1:C:51:ARG:HB3	2.22	0.40
1:C:532:ARG:HA	1:C:533:PRO:HD3	1.86	0.40
1:D:137:GLY:HA2	1:D:142:LEU:CD1	2.52	0.40
1:D:54:LEU:HA	1:D:54:LEU:HD23	1.88	0.40
1:A:103:ARG:N	1:A:104:PRO:CD	2.84	0.40
1:A:288:GLU:HB2	1:A:289:PRO:HD3	2.02	0.40
1:B:171:PHE:O	1:B:175:LYS:HG2	2.21	0.40
1:B:287:GLN:HA	1:B:287:GLN:NE2	2.36	0.40
1:B:288:GLU:CD	1:B:420:SER:HG	2.23	0.40
1:B:220:LYS:HG2	1:B:503:PHE:CZ	2.56	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	482/543 (89%)	447 (93%)	30 (6%)	5 (1%)	15 37
1	B	477/543 (88%)	443 (93%)	29 (6%)	5 (1%)	15 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	476/543 (88%)	444 (93%)	28 (6%)	4 (1%)	19	43
1	D	482/543 (89%)	449 (93%)	28 (6%)	5 (1%)	15	37
All	All	1917/2172 (88%)	1783 (93%)	115 (6%)	19 (1%)	15	37

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	GLU
1	B	281	GLU
1	C	281	GLU
1	D	281	GLU
1	A	138	ALA
1	B	119	ALA
1	B	138	ALA
1	B	413	PRO
1	C	119	ALA
1	D	138	ALA
1	A	413	PRO
1	C	413	PRO
1	D	119	ALA
1	D	413	PRO
1	A	119	ALA
1	B	512	PRO
1	A	512	PRO
1	D	512	PRO
1	C	512	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/449 (90%)	377 (93%)	28 (7%)	15	35
1	B	402/449 (90%)	376 (94%)	26 (6%)	17	38
1	C	405/449 (90%)	379 (94%)	26 (6%)	17	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	405/449 (90%)	379 (94%)	26 (6%)	17	39
All	All	1617/1796 (90%)	1511 (93%)	106 (7%)	16	38

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	50	LEU
1	A	61	MET
1	A	63	LEU
1	A	81	GLN
1	A	105	GLN
1	A	135	ARG
1	A	170	ARG
1	A	206	MET
1	A	223	LEU
1	A	230	GLN
1	A	258	THR
1	A	273	ARG
1	A	280	ASP
1	A	287	GLN
1	A	313	ARG
1	A	328	VAL
1	A	330	ILE
1	A	359	GLU
1	A	367	ASP
1	A	390	ARG
1	A	411	THR
1	A	433	GLU
1	A	448	THR
1	A	461	GLU
1	A	472	ASP
1	A	501	GLU
1	A	528	LEU
1	B	44	LEU
1	B	50	LEU
1	B	61	MET
1	B	63	LEU
1	B	81	GLN
1	B	105	GLN
1	B	135	ARG
1	B	206	MET

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Mol	Chain	Res	Type
1	B	223	LEU
1	B	230	GLN
1	B	258	THR
1	B	273	ARG
1	B	280	ASP
1	B	287	GLN
1	B	313	ARG
1	B	328	VAL
1	B	330	ILE
1	B	359	GLU
1	B	367	ASP
1	B	390	ARG
1	B	411	THR
1	B	433	GLU
1	B	461	GLU
1	B	472	ASP
1	B	501	GLU
1	B	528	LEU
1	C	44	LEU
1	C	50	LEU
1	C	61	MET
1	C	63	LEU
1	C	81	GLN
1	C	105	GLN
1	C	135	ARG
1	C	170	ARG
1	C	206	MET
1	C	223	LEU
1	C	230	GLN
1	C	273	ARG
1	C	280	ASP
1	C	287	GLN
1	C	328	VAL
1	C	330	ILE
1	C	359	GLU
1	C	367	ASP
1	C	390	ARG
1	C	411	THR
1	C	433	GLU
1	C	448	THR
1	C	461	GLU
1	C	473	SER

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Mol	Chain	Res	Type
1	C	501	GLU
1	C	528	LEU
1	D	44	LEU
1	D	50	LEU
1	D	61	MET
1	D	63	LEU
1	D	81	GLN
1	D	105	GLN
1	D	135	ARG
1	D	206	MET
1	D	223	LEU
1	D	230	GLN
1	D	273	ARG
1	D	280	ASP
1	D	287	GLN
1	D	312	TYR
1	D	313	ARG
1	D	328	VAL
1	D	330	ILE
1	D	359	GLU
1	D	367	ASP
1	D	390	ARG
1	D	411	THR
1	D	433	GLU
1	D	461	GLU
1	D	472	ASP
1	D	501	GLU
1	D	528	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	118	GLN
1	A	160	GLN
1	A	268	ASN
1	A	287	GLN
1	A	304	HIS
1	B	81	GLN
1	B	118	GLN
1	B	268	ASN
1	B	287	GLN

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Mol	Chain	Res	Type
1	B	304	HIS
1	C	81	GLN
1	C	118	GLN
1	C	160	GLN
1	C	268	ASN
1	C	287	GLN
1	C	304	HIS
1	D	81	GLN
1	D	118	GLN
1	D	160	GLN
1	D	180	GLN
1	D	268	ASN
1	D	287	GLN
1	D	304	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	544	-	5,5,5	0.37	0	5,5,5	0.29	0
4	GOL	A	544	-	5,5,5	0.47	0	5,5,5	0.70	0
2	ADP	C	700	3	24,29,29	0.92	1 (4%)	29,45,45	1.41	5 (17%)
2	ADP	D	700	3	24,29,29	0.96	1 (4%)	29,45,45	1.37	4 (13%)
2	ADP	A	700	3	24,29,29	1.02	2 (8%)	29,45,45	1.24	4 (13%)
2	ADP	B	700	3	24,29,29	1.01	2 (8%)	29,45,45	1.24	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	544	-	-	4/4/4/4	-
4	GOL	A	544	-	-	4/4/4/4	-
2	ADP	C	700	3	-	0/12/32/32	0/3/3/3
2	ADP	D	700	3	-	0/12/32/32	0/3/3/3
2	ADP	A	700	3	-	0/12/32/32	0/3/3/3
2	ADP	B	700	3	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	700	ADP	C5-C4	2.70	1.48	1.40
2	A	700	ADP	C5-C4	2.69	1.48	1.40
2	B	700	ADP	C5-C4	2.67	1.48	1.40
2	C	700	ADP	C5-C4	2.40	1.47	1.40
2	A	700	ADP	C2-N3	2.20	1.35	1.32
2	B	700	ADP	C2-N3	2.02	1.35	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	700	ADP	N3-C2-N1	-3.78	122.77	128.68
2	D	700	ADP	N3-C2-N1	-3.33	123.47	128.68
2	A	700	ADP	N3-C2-N1	-2.75	124.39	128.68
2	D	700	ADP	C3'-C2'-C1'	2.72	105.08	100.98
2	B	700	ADP	N3-C2-N1	-2.67	124.50	128.68
2	A	700	ADP	PA-O3A-PB	-2.66	123.71	132.83
2	D	700	ADP	N6-C6-N1	2.60	123.96	118.57
2	C	700	ADP	PA-O3A-PB	-2.51	124.21	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	ADP	PA-O3A-PB	-2.41	124.57	132.83
2	B	700	ADP	O3A-PB-O1B	-2.39	97.95	111.19
2	A	700	ADP	C3'-C2'-C1'	2.35	104.51	100.98
2	A	700	ADP	C4-C5-N7	-2.25	107.06	109.40
2	B	700	ADP	N6-C6-N1	2.24	123.23	118.57
2	C	700	ADP	C2-N1-C6	2.14	122.42	118.75
2	C	700	ADP	O3A-PB-O1B	-2.11	99.51	111.19
2	C	700	ADP	O3B-PB-O1B	2.00	118.53	110.68

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	544	GOL	O1-C1-C2-C3
4	A	544	GOL	O1-C1-C2-C3
4	B	544	GOL	C1-C2-C3-O3
4	A	544	GOL	C1-C2-C3-O3
4	B	544	GOL	O1-C1-C2-O2
4	A	544	GOL	O2-C2-C3-O3
4	A	544	GOL	O1-C1-C2-O2
4	B	544	GOL	O2-C2-C3-O3

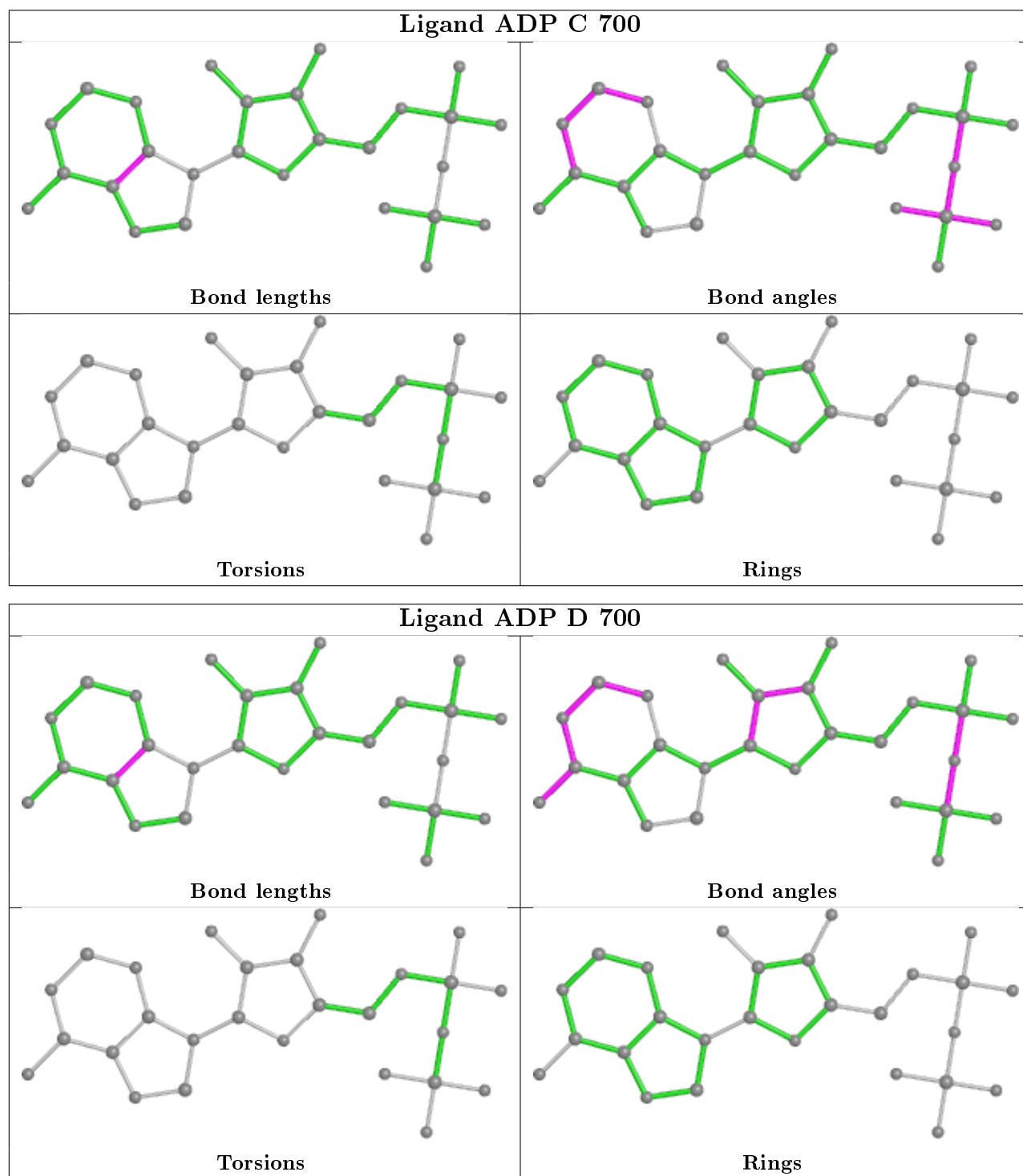
There are no ring outliers.

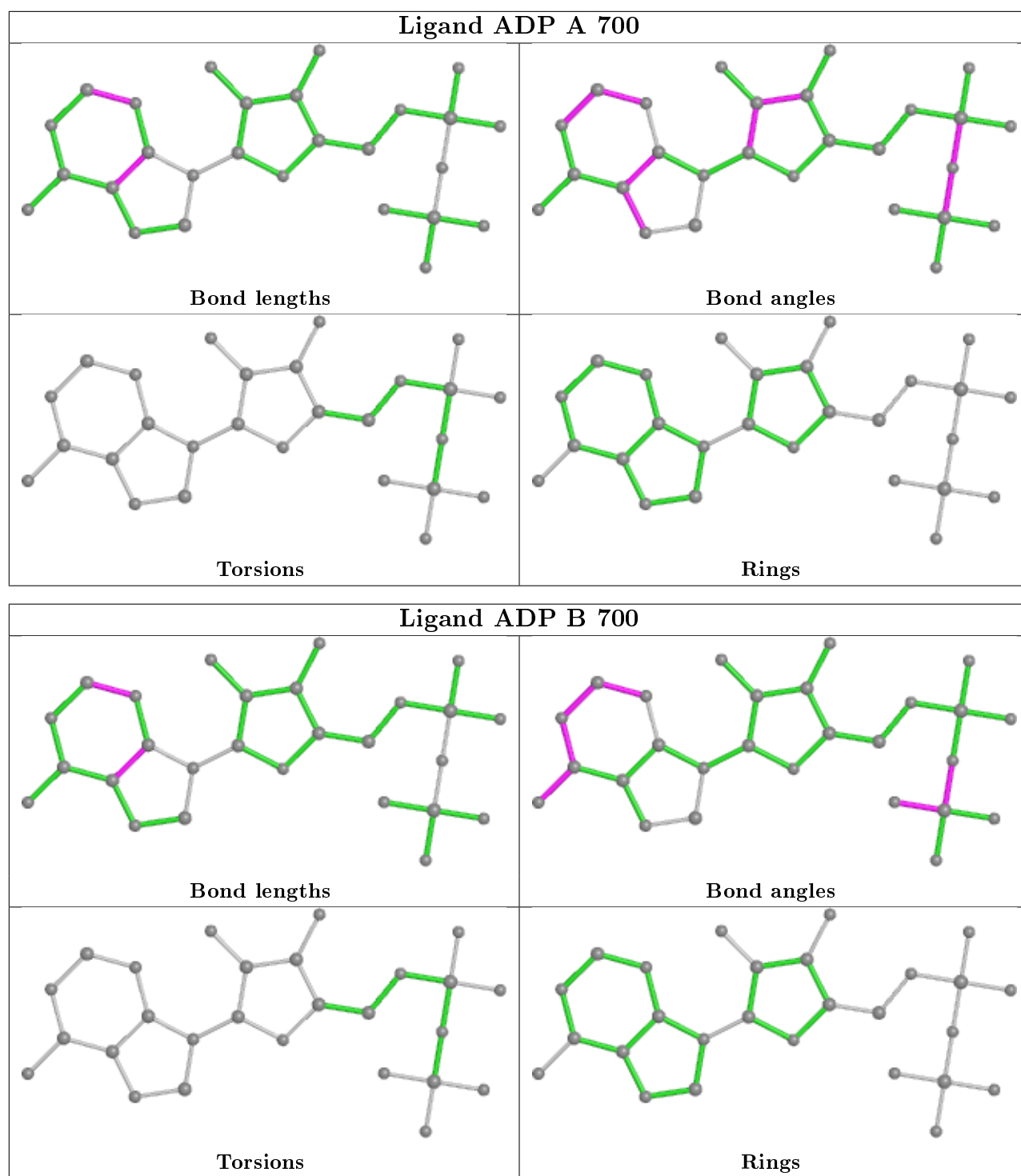
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	544	GOL	1	0
2	C	700	ADP	1	0
2	D	700	ADP	2	0
2	A	700	ADP	3	0
2	B	700	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	486/543 (89%)	0.12	23 (4%) 31 30	31, 59, 110, 132	1 (0%)
1	B	481/543 (88%)	0.01	20 (4%) 36 35	34, 60, 97, 126	1 (0%)
1	C	482/543 (88%)	-0.04	14 (2%) 51 52	31, 58, 93, 123	1 (0%)
1	D	486/543 (89%)	-0.01	23 (4%) 31 30	29, 56, 95, 120	1 (0%)
All	All	1935/2172 (89%)	0.02	80 (4%) 37 36	29, 58, 98, 132	4 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	490	VAL	5.3
1	D	281	GLU	4.5
1	D	493	VAL	4.0
1	D	495	PHE	4.0
1	B	281	GLU	3.9
1	D	492	GLY	3.8
1	A	140	ASP	3.8
1	C	281	GLU	3.7
1	B	283	ASN	3.6
1	D	282	ASP	3.5
1	A	99	ASP	3.4
1	B	341	ALA	3.3
1	B	282	ASP	3.1
1	A	472	ASP	3.1
1	D	279	VAL	3.1
1	A	132	ALA	3.0
1	B	101	ALA	2.9
1	D	453	ARG	2.9
1	C	315	LEU	2.9
1	A	375	LEU	2.8
1	C	282	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	101	ALA	2.8
1	B	279	VAL	2.8
1	D	312	TYR	2.8
1	D	491	LYS	2.8
1	B	495	PHE	2.7
1	C	133	ARG	2.7
1	A	378	THR	2.7
1	B	378	THR	2.7
1	C	33	ARG	2.7
1	B	377	VAL	2.6
1	C	377	VAL	2.6
1	D	472	ASP	2.6
1	B	195	ARG	2.6
1	D	33	ARG	2.6
1	D	283	ASN	2.6
1	C	379	LEU	2.6
1	A	116	GLU	2.6
1	C	135	ARG	2.6
1	A	283	ASN	2.5
1	A	317	PRO	2.5
1	B	317	PRO	2.5
1	C	376	GLY	2.5
1	A	131	VAL	2.5
1	A	453	ARG	2.4
1	C	283	ASN	2.4
1	C	378	THR	2.4
1	D	374	ALA	2.4
1	D	399	LYS	2.3
1	A	102	LEU	2.3
1	A	376	GLY	2.3
1	D	378	THR	2.3
1	B	374	ALA	2.3
1	B	320	VAL	2.3
1	A	115	LEU	2.3
1	A	315	LEU	2.3
1	C	134	ALA	2.3
1	C	317	PRO	2.2
1	D	375	LEU	2.2
1	D	341	ALA	2.2
1	A	135	ARG	2.2
1	B	375	LEU	2.2
1	C	375	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	190	PHE	2.2
1	A	118	GLN	2.2
1	A	119	ALA	2.2
1	B	371	ASP	2.2
1	A	320	VAL	2.2
1	B	414	ASP	2.1
1	D	314	ASP	2.1
1	D	319	ASN	2.1
1	B	192	VAL	2.1
1	D	315	LEU	2.1
1	B	280	ASP	2.1
1	A	490	VAL	2.1
1	B	312	TYR	2.1
1	B	314	ASP	2.1
1	D	331	SER	2.1
1	A	331	SER	2.0
1	A	112	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.

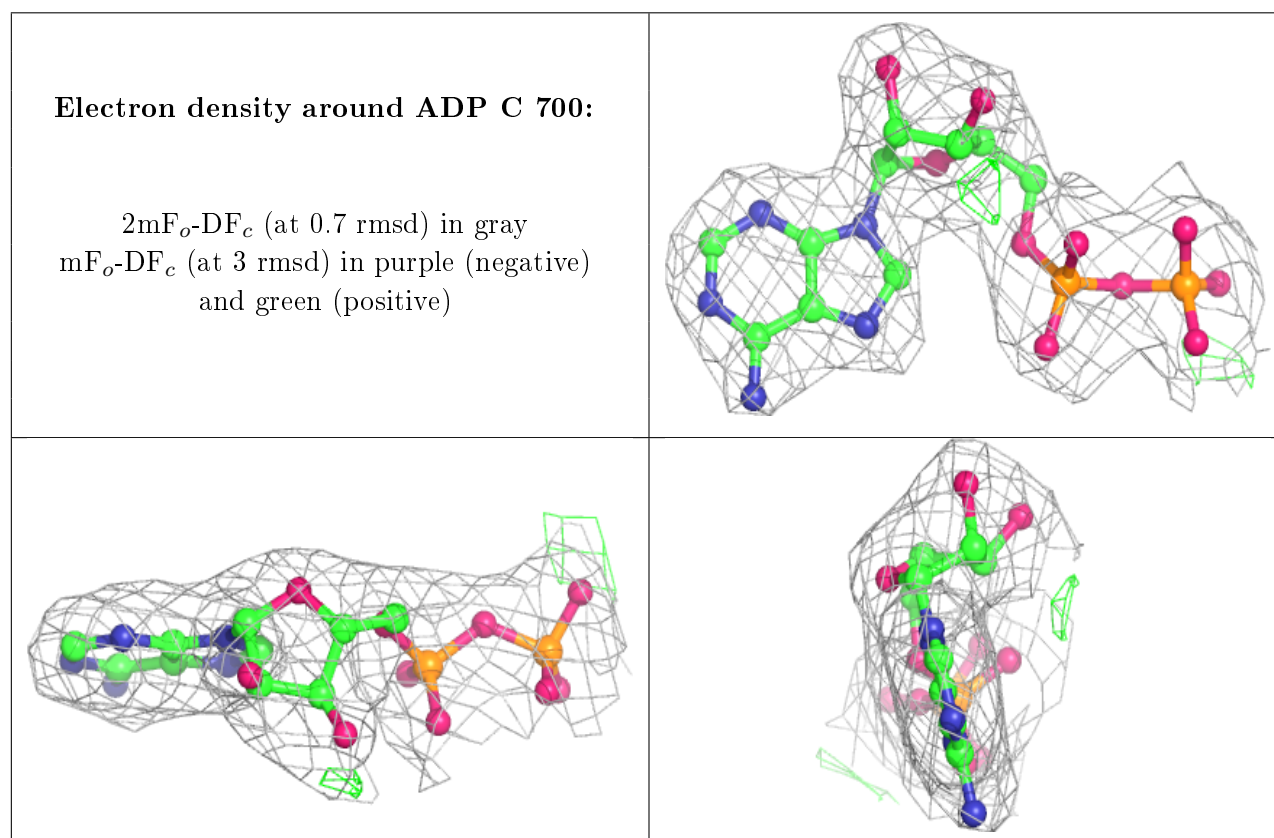
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	544	6/6	0.86	0.19	53,61,81,92	0
4	GOL	A	544	6/6	0.87	0.17	50,58,72,74	0
3	MG	B	800	1/1	0.92	0.15	43,43,43,43	0
3	MG	C	801	1/1	0.94	0.18	38,38,38,38	0
3	MG	C	800	1/1	0.96	0.17	29,29,29,29	0
3	MG	D	801	1/1	0.96	0.30	44,44,44,44	0

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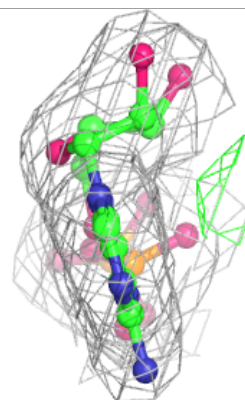
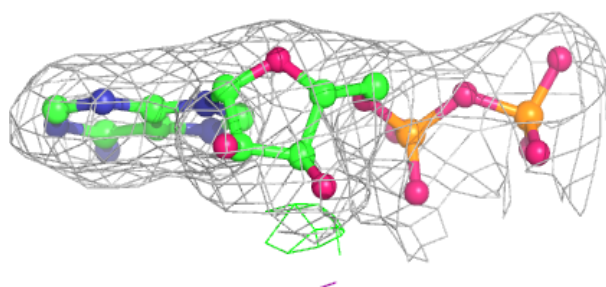
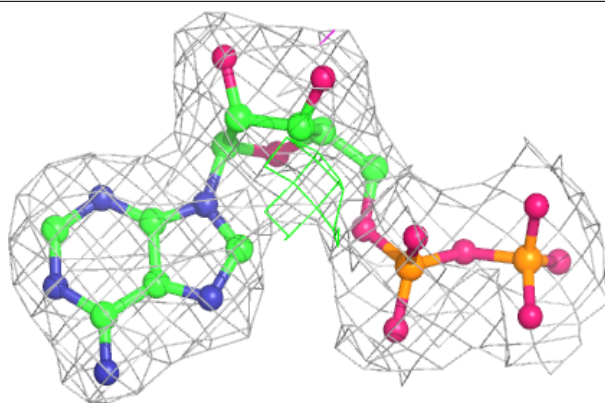
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	801	1/1	0.97	0.26	28,28,28,28	0
2	ADP	C	700	27/27	0.97	0.15	29,42,53,65	0
3	MG	A	800	1/1	0.98	0.12	23,23,23,23	0
3	MG	D	800	1/1	0.98	0.19	31,31,31,31	0
2	ADP	D	700	27/27	0.98	0.17	34,41,47,53	0
2	ADP	A	700	27/27	0.98	0.18	25,40,51,53	0
2	ADP	B	700	27/27	0.98	0.18	35,46,55,59	0
3	MG	B	801	1/1	0.98	0.30	51,51,51,51	0

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

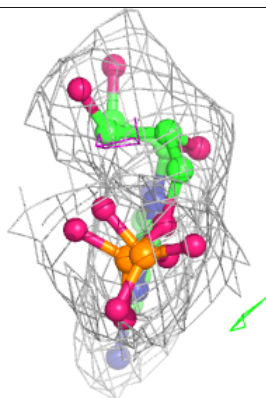
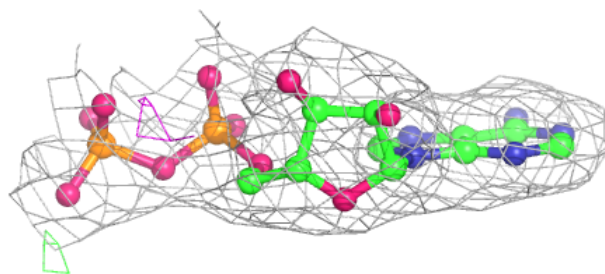
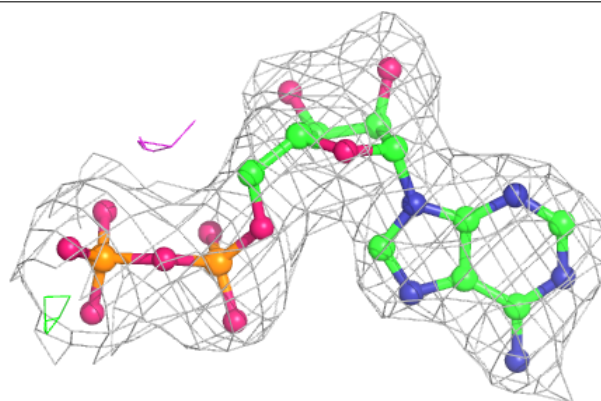


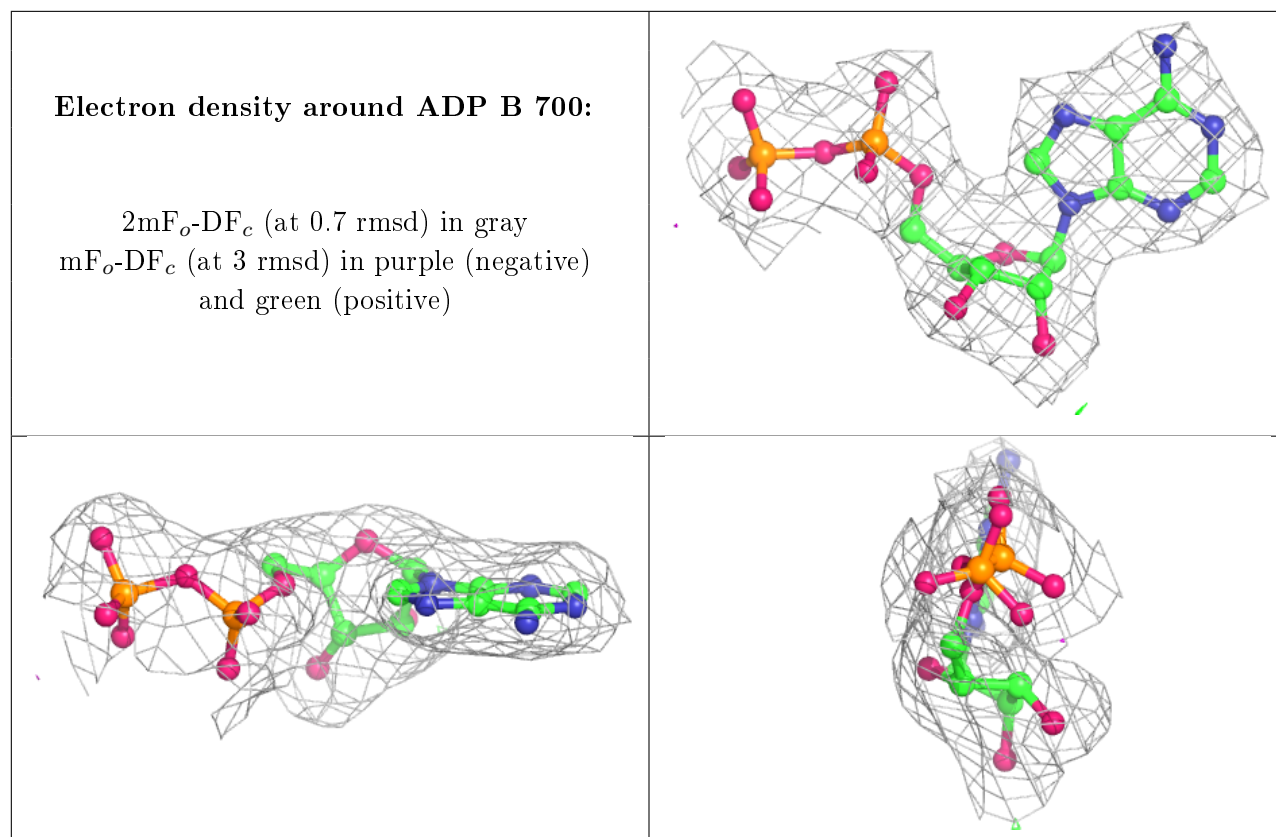
Electron density around ADP D 700:

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

**Electron density around ADP A 700:**

$2mF_o-DF_c$ (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.