Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:46 PM BST

PDB ID	:	6JIL
Title	:	Crystal structure of D-cycloserine synthetase DcsG
Authors	:	Matoba, Y.; Sugiyama, M.
Deposited on	:	2019-02-22
Resolution	:	2.32 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:

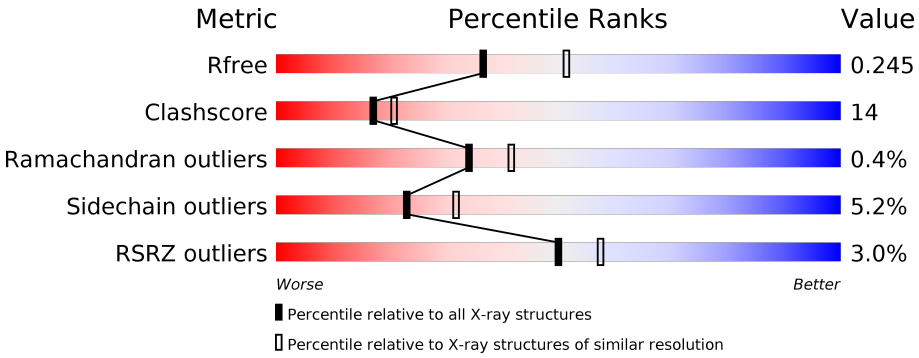
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 <=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	307	4% 73% 21%
1	B	307	2% 70% 25%
1	C	307	3% 72% 21%
1	D	307	3% 65% 29%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TLA	B	402	-	-	-	X
2	TLA	C	401	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10157 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 Cycloserine biosynthesis protein DcsG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	Se	0	0	0
			2290	1449	403	426	6	6			
1	B	298	Total	C	N	O	S	Se	0	0	0
			2298	1454	404	427	6	7			
1	C	298	Total	C	N	O	S	Se	0	0	0
			2298	1454	404	427	6	7			
1	D	298	Total	C	N	O	S	Se	0	0	0
			2298	1454	404	427	6	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	LEU	-	expression tag	UNP D2Z030
A	301	GLU	-	expression tag	UNP D2Z030
A	302	HIS	-	expression tag	UNP D2Z030
A	303	HIS	-	expression tag	UNP D2Z030
A	304	HIS	-	expression tag	UNP D2Z030
A	305	HIS	-	expression tag	UNP D2Z030
A	306	HIS	-	expression tag	UNP D2Z030
A	307	HIS	-	expression tag	UNP D2Z030
B	300	LEU	-	expression tag	UNP D2Z030
B	301	GLU	-	expression tag	UNP D2Z030
B	302	HIS	-	expression tag	UNP D2Z030
B	303	HIS	-	expression tag	UNP D2Z030
B	304	HIS	-	expression tag	UNP D2Z030
B	305	HIS	-	expression tag	UNP D2Z030
B	306	HIS	-	expression tag	UNP D2Z030
B	307	HIS	-	expression tag	UNP D2Z030
C	300	LEU	-	expression tag	UNP D2Z030
C	301	GLU	-	expression tag	UNP D2Z030
C	302	HIS	-	expression tag	UNP D2Z030
C	303	HIS	-	expression tag	UNP D2Z030
C	304	HIS	-	expression tag	UNP D2Z030

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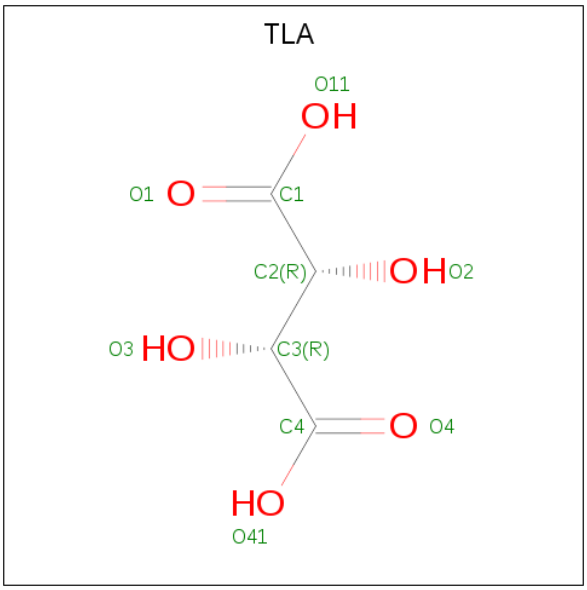
Chain	Residue	Modelled	Actual	Comment	Reference
C	305	HIS	-	expression tag	UNP D2Z030
C	306	HIS	-	expression tag	UNP D2Z030
C	307	HIS	-	expression tag	UNP D2Z030
D	300	LEU	-	expression tag	UNP D2Z030
D	301	GLU	-	expression tag	UNP D2Z030
D	302	HIS	-	expression tag	UNP D2Z030
D	303	HIS	-	expression tag	UNP D2Z030
D	304	HIS	-	expression tag	UNP D2Z030
D	305	HIS	-	expression tag	UNP D2Z030
D	306	HIS	-	expression tag	UNP D2Z030
D	307	HIS	-	expression tag	UNP D2Z030

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 4 6	0	0
2	A	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	C	1	Total C O 10 4 6	0	0

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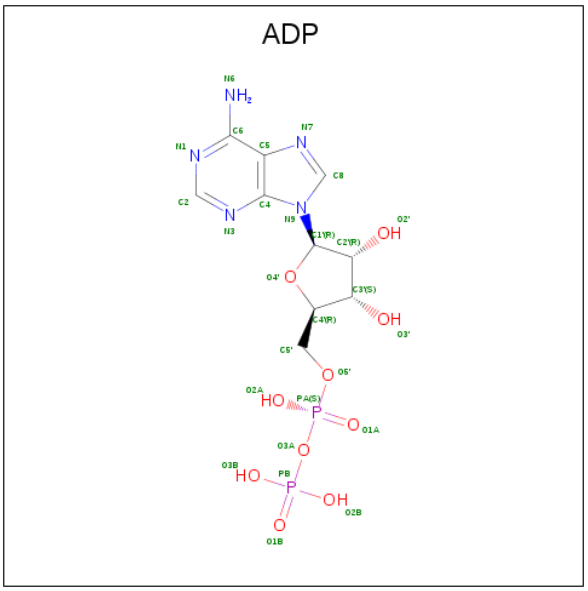
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 10 4 6	0	0
2	C	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0

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



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Mg 2 2	0	0

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

- Molecule 5 is water.

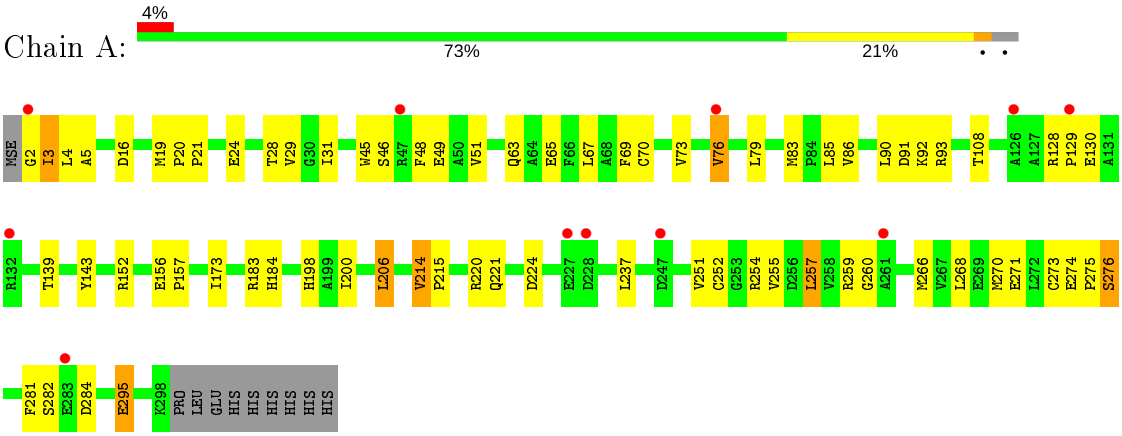
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	217	Total O 217 217	0	0
5	B	199	Total O 199 199	0	0
5	C	171	Total O 171 171	0	0
5	D	169	Total O 169 169	0	0

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.

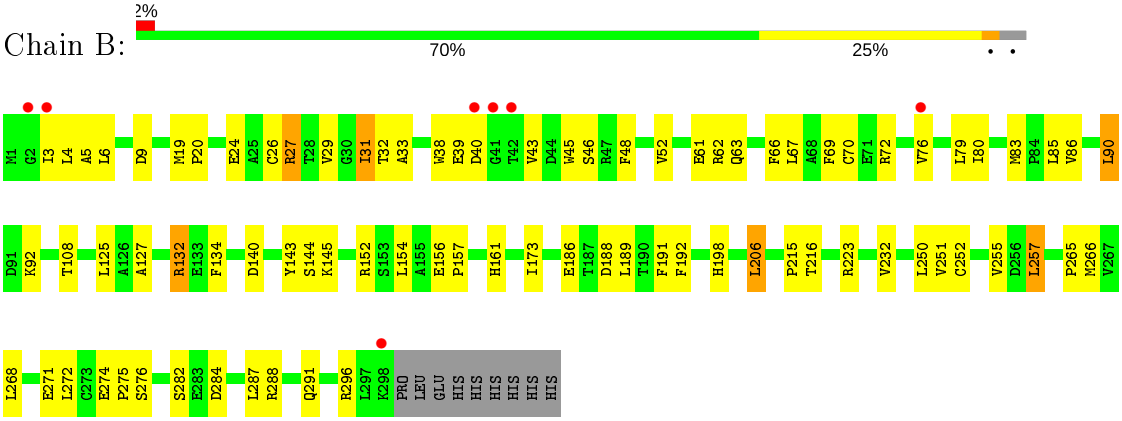
- Molecule 1: Cycloserine biosynthesis protein DcsG

Chain A:



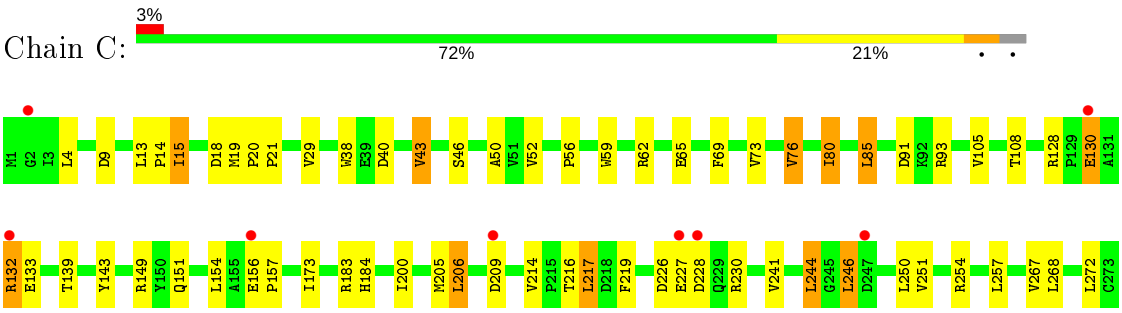
- Molecule 1: Cycloserine biosynthesis protein DcsG

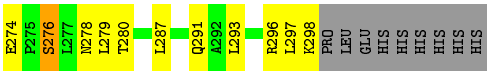
Chain B:



- Molecule 1: Cycloserine biosynthesis protein DcsG

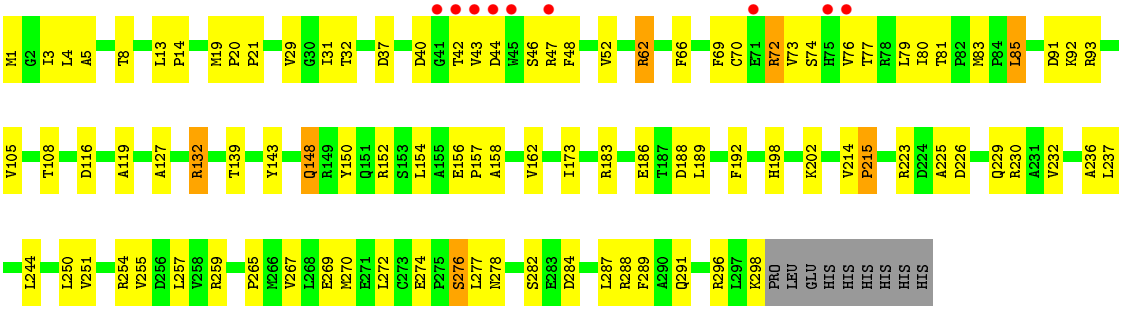
Chain C:





- Molecule 1: Cycloserine biosynthesis protein DcsG

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.45Å 120.73Å 102.81Å 90.00° 101.01° 90.00°	Depositor
Resolution (Å)	29.76 – 2.32 32.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.76-2.32) 94.7 (32.56-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.31Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.195 , 0.251 0.190 , 0.245	Depositor DCC
R_{free} test set	2862 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.4	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	10157	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.06% 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: TLA, 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	0.33	0/2337	0.63	1/3180 (0.0%)
1	B	0.32	0/2345	0.62	1/3190 (0.0%)
1	C	0.31	0/2345	0.60	1/3190 (0.0%)
1	D	0.32	0/2345	0.60	1/3190 (0.0%)
All	All	0.32	0/9372	0.61	4/12750 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	276	SER	N-CA-C	-5.87	95.16	111.00
1	A	276	SER	N-CA-C	-5.83	95.25	111.00
1	D	276	SER	N-CA-C	-5.50	96.14	111.00
1	B	276	SER	N-CA-C	-5.14	97.13	111.00

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	2290	0	2258	57	0
1	B	2298	0	2270	61	0
1	C	2298	0	2270	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2298	0	2270	82	0
2	A	20	0	8	1	0
2	B	30	0	12	3	0
2	C	30	0	12	0	0
2	D	20	0	8	3	0
3	A	27	0	12	3	0
3	B	27	0	12	2	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
5	A	217	0	0	4	0
5	B	199	0	0	4	0
5	C	171	0	0	6	0
5	D	169	0	0	5	0
All	All	10157	0	9156	258	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 14.

All (258) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:SER:HA	1:C:76:VAL:HG13	1.58	0.86
1:D:72:ARG:HB2	1:D:72:ARG:HH11	1.40	0.85
1:A:79:LEU:HD13	1:A:83:MSE:HE3	1.57	0.85
1:A:79:LEU:CD1	1:A:83:MSE:HE3	2.06	0.84
1:D:156:GLU:HB3	1:D:157:PRO:HD3	1.57	0.84
1:C:244:LEU:HB3	1:C:246:LEU:HD13	1.60	0.84
1:A:83:MSE:HA	1:A:83:MSE:HE2	1.63	0.81
1:D:132:ARG:HA	1:D:132:ARG:HE	1.46	0.80
1:B:70:CYS:HB3	1:B:83:MSE:HE1	1.62	0.80
1:D:70:CYS:HB3	1:D:83:MSE:HE1	1.64	0.79
1:B:79:LEU:CD1	1:B:83:MSE:HE3	2.13	0.78
1:D:79:LEU:CD1	1:D:83:MSE:HE3	2.16	0.75
1:D:69:PHE:HA	1:D:72:ARG:HH12	1.51	0.74
1:A:139:THR:HG22	1:A:173:ILE:HG13	1.70	0.73
1:C:297:LEU:O	1:C:298:LYS:HB2	1.89	0.72
1:D:69:PHE:HA	1:D:72:ARG:NH1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:MSE:HE3	5:B:511:HOH:O	1.89	0.72
1:C:250:LEU:HD13	1:C:272:LEU:HD22	1.70	0.72
1:B:29:VAL:HG23	1:B:31:ILE:HG23	1.72	0.71
1:C:156:GLU:HB3	1:C:157:PRO:HD3	1.71	0.71
1:B:31:ILE:HD11	1:B:33:ALA:HB2	1.72	0.70
1:C:280:THR:HG22	5:C:526:HOH:O	1.91	0.70
1:A:237:LEU:HD23	1:A:270:MSE:HE2	1.75	0.69
1:B:26:CYS:HB3	1:B:31:ILE:HG13	1.75	0.69
1:C:69:PHE:O	1:C:73:VAL:HG23	1.94	0.68
1:D:80:ILE:CG2	1:D:251:VAL:HG21	2.24	0.67
1:B:251:VAL:HG22	1:B:296:ARG:CZ	2.24	0.67
1:D:44:ASP:O	1:D:47:ARG:HG2	1.95	0.67
1:B:70:CYS:HB3	1:B:83:MSE:CE	2.26	0.66
1:D:251:VAL:HG22	1:D:296:ARG:CZ	2.25	0.66
1:A:3:ILE:HD11	5:A:574:HOH:O	1.94	0.66
1:B:83:MSE:HA	1:B:83:MSE:HE2	1.79	0.65
1:C:80:ILE:HG23	1:C:251:VAL:HG21	1.77	0.65
1:C:139:THR:HG22	1:C:173:ILE:HG13	1.78	0.64
1:D:72:ARG:HH11	1:D:72:ARG:CB	2.11	0.63
1:A:69:PHE:O	1:A:73:VAL:HG23	1.98	0.63
1:D:79:LEU:HD13	1:D:83:MSE:HE3	1.79	0.63
1:C:46:SER:CA	1:C:76:VAL:HG13	2.29	0.62
1:A:156:GLU:HB3	1:A:157:PRO:HD3	1.80	0.62
1:D:83:MSE:HE2	1:D:83:MSE:HA	1.81	0.62
1:D:46:SER:OG	1:D:76:VAL:HG21	2.00	0.62
1:B:108:THR:HG23	1:B:173:ILE:HG23	1.81	0.62
1:B:156:GLU:HB3	1:B:157:PRO:HD3	1.81	0.61
1:A:255:VAL:HG22	1:A:270:MSE:HE3	1.82	0.61
1:A:206:LEU:HD22	3:A:403:ADP:H1'	1.82	0.61
1:D:232:VAL:HG21	1:D:265:PRO:HG2	1.83	0.60
1:D:154:LEU:O	1:D:157:PRO:HD2	2.01	0.60
1:D:52:VAL:HG22	1:D:80:ILE:HG13	1.81	0.60
1:B:250:LEU:HD13	1:B:272:LEU:HD22	1.83	0.60
1:D:4:LEU:HD23	1:D:5:ALA:N	2.17	0.60
3:D:403:ADP:O3B	3:D:403:ADP:O2A	2.20	0.60
1:D:74:SER:HB3	1:D:79:LEU:HD11	1.84	0.59
1:D:251:VAL:HG23	5:D:522:HOH:O	2.02	0.59
1:C:227:GLU:HG2	5:C:547:HOH:O	2.02	0.59
1:C:91:ASP:OD2	1:C:93:ARG:HD3	2.04	0.58
1:D:29:VAL:HG23	1:D:31:ILE:HG13	1.83	0.58
1:C:143:TYR:CZ	1:C:214:VAL:HG13	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:LEU:HD23	1:D:270:MSE:HE2	1.85	0.58
1:B:287:LEU:O	1:B:291:GLN:HG3	2.04	0.58
1:D:223:ARG:HD3	5:D:568:HOH:O	2.03	0.57
1:A:91:ASP:OD1	1:A:93:ARG:HD3	2.03	0.57
1:B:80:ILE:CG2	1:B:251:VAL:HG21	2.35	0.57
1:D:70:CYS:HB3	1:D:83:MSE:CE	2.34	0.57
1:A:108:THR:HG23	1:A:173:ILE:HG23	1.86	0.56
1:B:284:ASP:HA	5:B:614:HOH:O	2.05	0.56
1:C:183:ARG:HG3	1:C:184:HIS:ND1	2.20	0.56
1:C:85:LEU:HA	1:C:244:LEU:HD21	1.88	0.56
1:C:230:ARG:HD2	5:C:513:HOH:O	2.04	0.56
1:C:50:ALA:HB1	1:C:80:ILE:HD13	1.85	0.56
1:A:70:CYS:HB3	1:A:83:MSE:HE1	1.88	0.56
1:C:128:ARG:HA	1:C:130:GLU:OE2	2.06	0.56
1:D:156:GLU:HB3	1:D:157:PRO:CD	2.35	0.55
1:D:40:ASP:O	1:D:43:VAL:HG12	2.07	0.55
1:C:80:ILE:CG2	1:C:251:VAL:HG21	2.37	0.55
1:D:62:ARG:NH1	1:D:62:ARG:HB3	2.22	0.55
1:D:229:GLN:HB3	1:D:257:LEU:HD12	1.88	0.55
1:B:186:GLU:HG2	5:B:529:HOH:O	2.05	0.55
1:B:24:GLU:OE1	1:B:27:ARG:NH2	2.38	0.55
1:D:19:MSE:HB3	1:D:20:PRO:HD3	1.88	0.55
1:B:198:HIS:CG	1:B:282:SER:HB3	2.42	0.54
1:D:198:HIS:CG	1:D:282:SER:HB3	2.43	0.54
1:A:260:GLY:HA3	1:A:266:MSE:HE3	1.89	0.54
1:D:72:ARG:HB2	1:D:72:ARG:NH1	2.17	0.54
1:A:83:MSE:CE	1:A:86:VAL:HG21	2.38	0.54
1:A:183:ARG:HH11	1:A:184:HIS:CE1	2.26	0.53
1:C:50:ALA:HB1	1:C:80:ILE:CD1	2.39	0.52
1:D:116:ASP:HB3	1:D:119:ALA:HB3	1.91	0.52
1:D:43:VAL:HA	5:D:561:HOH:O	2.10	0.52
1:B:215:PRO:HG3	2:B:403:TLA:H2	1.91	0.51
1:A:86:VAL:O	1:A:90:LEU:HD13	2.10	0.51
1:B:132:ARG:O	1:B:152:ARG:HG3	2.10	0.51
1:B:232:VAL:HG21	1:B:257:LEU:HG	1.93	0.51
1:B:46:SER:HB3	1:B:76:VAL:HG21	1.92	0.51
1:D:5:ALA:HB2	1:D:48:PHE:CD2	2.46	0.51
2:D:402:TLA:H2	5:D:555:HOH:O	2.10	0.51
1:C:91:ASP:OD2	1:C:93:ARG:HB2	2.10	0.51
1:A:152:ARG:HD3	5:A:658:HOH:O	2.11	0.51
1:A:3:ILE:HG23	1:A:48:PHE:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLU:HB3	1:B:275:PRO:HB3	1.92	0.51
1:D:76:VAL:HG22	1:D:76:VAL:O	2.11	0.51
1:A:63:GLN:O	1:A:67:LEU:HD13	2.10	0.50
1:D:250:LEU:HD13	1:D:272:LEU:HD22	1.93	0.50
1:B:132:ARG:HE	1:B:132:ARG:HA	1.75	0.50
1:D:154:LEU:C	1:D:157:PRO:HD2	2.32	0.50
1:D:1:MSE:HE3	1:D:298:LYS:HB3	1.94	0.50
1:A:19:MSE:HB3	1:A:20:PRO:HD3	1.94	0.50
1:B:31:ILE:HD12	1:B:31:ILE:C	2.32	0.50
1:A:2:GLY:HA2	1:A:49:GLU:HB2	1.94	0.50
1:D:287:LEU:O	1:D:291:GLN:HG3	2.11	0.50
1:B:232:VAL:HG11	1:B:265:PRO:HG2	1.94	0.50
1:A:46:SER:HB3	1:A:76:VAL:CG2	2.42	0.49
1:A:5:ALA:HB3	1:A:51:VAL:HG22	1.94	0.49
1:C:132:ARG:HE	1:C:132:ARG:HA	1.77	0.49
1:D:132:ARG:HH21	1:D:152:ARG:HD3	1.76	0.49
1:B:19:MSE:HB3	1:B:20:PRO:HD3	1.95	0.49
1:C:15:ILE:HG23	1:C:15:ILE:O	2.12	0.49
1:D:226:ASP:O	1:D:230:ARG:HG2	2.11	0.49
1:D:40:ASP:OD2	1:D:42:THR:HB	2.13	0.49
1:D:105:VAL:HG12	1:D:267:VAL:HB	1.94	0.49
1:A:200:ILE:HD12	1:A:220:ARG:HB3	1.94	0.49
1:C:29:VAL:HG12	1:C:29:VAL:O	2.13	0.49
1:D:148:GLN:HB3	1:D:150:TYR:CE1	2.48	0.48
1:A:251:VAL:HG23	1:A:252:CYS:N	2.29	0.48
1:A:3:ILE:CG2	1:A:48:PHE:CD2	2.96	0.48
1:B:206:LEU:HD22	3:B:404:ADP:H1'	1.95	0.48
1:C:149:ARG:HD2	1:C:206:LEU:HB3	1.95	0.48
1:C:287:LEU:O	1:C:291:GLN:HG3	2.13	0.48
1:D:192:PHE:CE2	1:D:289:PHE:HB2	2.48	0.48
1:A:83:MSE:CE	1:A:83:MSE:HA	2.40	0.48
1:D:225:ALA:HB3	1:D:230:ARG:HD3	1.95	0.48
1:D:284:ASP:O	1:D:288:ARG:HG3	2.13	0.48
1:C:13:LEU:N	1:C:14:PRO:HD2	2.29	0.48
1:D:80:ILE:HG22	1:D:251:VAL:HG21	1.96	0.48
1:D:189:LEU:HD12	1:D:189:LEU:N	2.28	0.48
1:C:4:LEU:HD11	1:C:52:VAL:HG23	1.95	0.48
1:C:62:ARG:HB2	1:C:65:GLU:HB2	1.96	0.48
1:A:24:GLU:O	1:A:28:THR:HG23	2.13	0.47
1:B:127:ALA:HB3	1:D:127:ALA:HB3	1.95	0.47
1:A:284:ASP:HA	5:A:629:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TRP:CD1	2:A:401:TLA:H3	2.49	0.47
1:B:63:GLN:O	1:B:67:LEU:HD23	2.15	0.47
1:D:4:LEU:HD21	1:D:52:VAL:CG2	2.44	0.47
1:A:237:LEU:CD2	1:A:270:MSE:HE2	2.42	0.47
1:D:186:GLU:HG2	5:D:543:HOH:O	2.14	0.47
1:D:259:ARG:HH12	1:D:265:PRO:HD3	1.80	0.47
1:D:255:VAL:HG22	1:D:270:MSE:HE3	1.95	0.47
1:D:143:TYR:CE1	1:D:215:PRO:HG2	2.49	0.47
1:D:237:LEU:CD2	1:D:270:MSE:HE2	2.45	0.47
1:C:9:ASP:HB3	1:C:38:TRP:CD1	2.50	0.46
1:D:156:GLU:CB	1:D:157:PRO:HD3	2.38	0.46
1:D:158:ALA:O	1:D:162:VAL:HG23	2.15	0.46
1:B:61:GLU:HG2	1:B:145:LYS:HE3	1.96	0.46
1:B:39:GLU:OE1	1:B:62:ARG:CZ	2.63	0.46
1:C:251:VAL:HG22	1:C:296:ARG:CZ	2.45	0.46
1:C:226:ASP:HB2	5:C:547:HOH:O	2.15	0.46
1:D:81:THR:HB	1:D:85:LEU:HD13	1.97	0.46
1:B:79:LEU:HD11	1:B:83:MSE:HE3	1.94	0.46
1:A:46:SER:HB3	1:A:76:VAL:HG21	1.97	0.46
1:D:20:PRO:HB2	1:D:21:PRO:CD	2.46	0.46
1:D:73:VAL:O	1:D:77:THR:HG22	2.15	0.46
1:C:205:MSE:HE1	1:C:219:PHE:CD2	2.51	0.46
1:D:236:ALA:C	1:D:270:MSE:HE1	2.35	0.46
1:D:269:GLU:HG2	1:D:270:MSE:N	2.30	0.45
1:B:255:VAL:HG12	1:B:257:LEU:CD1	2.46	0.45
1:B:5:ALA:HB2	1:B:48:PHE:CG	2.51	0.45
1:A:259:ARG:HD2	5:A:659:HOH:O	2.16	0.45
1:B:189:LEU:N	1:B:189:LEU:HD12	2.31	0.45
1:C:19:MSE:HB3	1:C:20:PRO:HD3	1.99	0.45
1:A:198:HIS:CG	1:A:282:SER:HB3	2.50	0.45
1:C:40:ASP:O	1:C:43:VAL:HG13	2.17	0.45
1:D:72:ARG:NH1	2:D:401:TLA:H2	2.32	0.45
1:A:65:GLU:N	1:A:65:GLU:OE2	2.46	0.45
1:C:251:VAL:HG22	1:C:296:ARG:NH1	2.32	0.45
1:B:127:ALA:CB	1:D:127:ALA:HB3	2.47	0.45
1:A:91:ASP:OD2	1:A:139:THR:HB	2.17	0.44
3:B:404:ADP:O2A	3:B:404:ADP:O1B	2.34	0.44
1:B:143:TYR:O	1:B:144:SER:HB2	2.16	0.44
1:B:6:LEU:HD23	1:B:52:VAL:CG1	2.46	0.44
1:D:108:THR:HG23	1:D:173:ILE:HG23	2.00	0.44
1:D:254:ARG:HD3	1:D:276:SER:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:HG23	1:A:48:PHE:CD2	2.51	0.44
1:C:18:ASP:HB3	1:C:279:LEU:HD12	2.00	0.44
1:D:188:ASP:OD2	1:D:202:LYS:HE3	2.18	0.44
1:D:4:LEU:HD21	1:D:52:VAL:HG23	2.00	0.44
1:A:206:LEU:HD22	3:A:403:ADP:C1'	2.47	0.44
1:B:63:GLN:N	1:B:63:GLN:OE1	2.38	0.44
1:D:72:ARG:HH11	2:D:401:TLA:H2	1.82	0.44
1:C:241:VAL:HG13	1:C:246:LEU:HB2	2.00	0.43
1:C:254:ARG:HD3	1:C:276:SER:O	2.17	0.43
1:B:9:ASP:HB3	1:B:38:TRP:CD1	2.53	0.43
1:C:108:THR:HG23	1:C:173:ILE:HG23	2.00	0.43
1:C:298:LYS:HA	1:C:298:LYS:HD2	1.85	0.43
3:A:403:ADP:O1B	3:A:403:ADP:O2A	2.35	0.43
1:B:5:ALA:HB2	1:B:48:PHE:CD2	2.53	0.43
1:A:3:ILE:CG2	1:A:48:PHE:HD2	2.30	0.43
1:B:271:GLU:OE1	1:B:275:PRO:HA	2.19	0.43
1:B:72:ARG:HB3	2:B:402:TLA:H2	2.01	0.43
1:C:154:LEU:O	1:C:157:PRO:HD2	2.18	0.43
1:A:20:PRO:HB2	1:A:21:PRO:CD	2.48	0.43
1:A:5:ALA:HB2	1:A:48:PHE:CD2	2.53	0.43
1:B:125:LEU:HD21	1:B:134:PHE:CD2	2.54	0.43
1:B:46:SER:HB3	1:B:76:VAL:CG2	2.49	0.43
1:C:130:GLU:CD	1:C:130:GLU:H	2.21	0.43
1:C:206:LEU:HD22	3:C:404:ADP:H1'	2.01	0.43
1:B:63:GLN:HG2	1:B:140:ASP:OD1	2.19	0.42
1:A:128:ARG:O	1:A:152:ARG:NH2	2.52	0.42
1:B:154:LEU:O	1:B:157:PRO:HD2	2.20	0.42
1:B:83:MSE:CE	1:B:86:VAL:HG21	2.49	0.42
1:C:200:ILE:HD13	1:C:278:ASN:CG	2.40	0.42
1:C:56:PRO:O	1:C:59:TRP:HD1	2.01	0.42
1:A:29:VAL:HG23	1:A:31:ILE:HG12	2.01	0.42
1:D:52:VAL:HG22	1:D:80:ILE:CG1	2.48	0.42
1:C:209:ASP:C	1:C:209:ASP:OD2	2.58	0.42
1:B:3:ILE:HA	1:B:32:THR:O	2.20	0.42
1:D:259:ARG:NH1	1:D:265:PRO:HD3	2.34	0.42
1:B:45:TRP:CD1	2:B:402:TLA:H3	2.55	0.42
1:C:183:ARG:HG3	1:C:184:HIS:CE1	2.54	0.42
1:D:20:PRO:HB2	1:D:21:PRO:HD3	2.01	0.42
1:D:3:ILE:HG12	1:D:32:THR:CG2	2.50	0.42
1:B:284:ASP:O	1:B:288:ARG:HG3	2.20	0.42
1:C:20:PRO:HB2	1:C:21:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:LEU:HB3	1:D:14:PRO:HD3	2.00	0.42
1:B:192:PHE:HA	1:B:251:VAL:O	2.20	0.42
1:B:223:ARG:HD3	5:B:623:HOH:O	2.19	0.42
1:C:105:VAL:HG12	1:C:267:VAL:HB	2.02	0.42
1:A:221:GLN:HA	1:A:281:PHE:HE2	1.85	0.41
1:D:91:ASP:OD2	1:D:139:THR:HB	2.20	0.41
1:A:255:VAL:HG12	1:A:257:LEU:CD1	2.50	0.41
1:A:295:GLU:OE1	1:A:295:GLU:HA	2.21	0.41
1:B:186:GLU:OE1	1:B:188:ASP:OD1	2.38	0.41
1:C:251:VAL:HG11	1:C:293:LEU:HD23	2.01	0.41
1:D:277:LEU:O	1:D:278:ASN:HB2	2.20	0.41
1:A:20:PRO:HB2	1:A:21:PRO:HD3	2.03	0.41
1:A:254:ARG:HD3	1:A:276:SER:O	2.20	0.41
1:A:46:SER:CB	1:A:76:VAL:HG22	2.50	0.41
1:B:191:PHE:O	1:B:252:CYS:HA	2.19	0.41
1:A:90:LEU:HD11	1:A:273:CYS:SG	2.60	0.41
1:B:127:ALA:HB3	1:D:127:ALA:CB	2.50	0.41
1:A:271:GLU:HB3	1:A:275:PRO:HB3	2.02	0.41
1:C:93:ARG:NH1	5:C:512:HOH:O	2.54	0.41
1:A:129:PRO:HA	1:A:152:ARG:HH22	1.86	0.41
1:A:143:TYR:CZ	1:A:214:VAL:HG13	2.56	0.41
1:B:66:PHE:O	1:B:69:PHE:HB3	2.21	0.41
1:B:61:GLU:C	1:B:62:ARG:HG2	2.41	0.41
1:B:86:VAL:O	1:B:90:LEU:HB2	2.20	0.41
1:C:151:GLN:HG3	5:C:594:HOH:O	2.21	0.41
1:D:62:ARG:HB3	1:D:62:ARG:CZ	2.51	0.41
1:C:244:LEU:HB3	1:C:246:LEU:CD1	2.40	0.40
1:A:83:MSE:HE1	1:A:86:VAL:HG21	2.02	0.40
1:D:13:LEU:N	1:D:14:PRO:CD	2.84	0.40
1:A:183:ARG:NH1	1:A:184:HIS:CE1	2.87	0.40
1:B:40:ASP:OD1	1:B:43:VAL:HG23	2.21	0.40
1:C:133:GLU:HG2	1:C:151:GLN:HA	2.03	0.40
1:C:20:PRO:HB2	1:C:21:PRO:CD	2.50	0.40
1:D:8:THR:O	1:D:37:ASP:HA	2.21	0.40
1:A:16:ASP:OD2	1:A:19:MSE:HE2	2.22	0.40
1:D:66:PHE:O	1:D:69:PHE:HB3	2.21	0.40
1:C:217:LEU:HA	1:C:217:LEU:HD12	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/307 (96%)	285 (97%)	8 (3%)	2 (1%)	22	26
1	B	296/307 (96%)	285 (96%)	10 (3%)	1 (0%)	41	50
1	C	296/307 (96%)	280 (95%)	16 (5%)	0	100	100
1	D	296/307 (96%)	281 (95%)	13 (4%)	2 (1%)	22	26
All	All	1183/1228 (96%)	1131 (96%)	47 (4%)	5 (0%)	34	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	92	LYS
1	B	92	LYS
1	A	92	LYS
1	A	215	PRO
1	D	215	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/244 (99%)	229 (95%)	12 (5%)	24	34
1	B	242/244 (99%)	230 (95%)	12 (5%)	24	34
1	C	242/244 (99%)	226 (93%)	16 (7%)	16	22
1	D	242/244 (99%)	232 (96%)	10 (4%)	30	43
All	All	967/976 (99%)	917 (95%)	50 (5%)	23	32

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	4	LEU
1	A	76	VAL
1	A	85	LEU
1	A	130	GLU
1	A	206	LEU
1	A	214	VAL
1	A	224	ASP
1	A	257	LEU
1	A	268	LEU
1	A	274	GLU
1	A	295	GLU
1	B	4	LEU
1	B	27	ARG
1	B	31	ILE
1	B	85	LEU
1	B	90	LEU
1	B	132	ARG
1	B	161	HIS
1	B	206	LEU
1	B	216	THR
1	B	257	LEU
1	B	268	LEU
1	B	274	GLU
1	C	15	ILE
1	C	43	VAL
1	C	76	VAL
1	C	80	ILE
1	C	85	LEU
1	C	130	GLU
1	C	132	ARG
1	C	206	LEU
1	C	216	THR
1	C	217	LEU
1	C	228	ASP
1	C	244	LEU
1	C	246	LEU
1	C	257	LEU
1	C	268	LEU
1	C	274	GLU
1	D	62	ARG
1	D	72	ARG

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Mol	Chain	Res	Type
1	D	85	LEU
1	D	93	ARG
1	D	132	ARG
1	D	148	GLN
1	D	183	ARG
1	D	214	VAL
1	D	244	LEU
1	D	274	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	151	GLN
1	A	184	HIS
1	B	101	HIS
1	B	161	HIS
1	C	101	HIS
1	C	151	GLN
1	D	148	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 9 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	D	403	4	24,29,29	1.28	2 (8%)	29,45,45	1.65	5 (17%)
2	TLA	B	403	4	3,9,9	0.51	0	6,12,12	1.24	2 (33%)
2	TLA	C	401	-	3,9,9	0.39	0	6,12,12	0.87	0
2	TLA	A	401	-	3,9,9	0.14	0	6,12,12	0.93	0
3	ADP	A	403	4	24,29,29	1.34	3 (12%)	29,45,45	1.58	4 (13%)
3	ADP	C	404	4	24,29,29	1.22	2 (8%)	29,45,45	1.64	3 (10%)
2	TLA	C	402	-	3,9,9	0.31	0	6,12,12	0.88	0
3	ADP	B	404	4	24,29,29	1.36	3 (12%)	29,45,45	1.58	4 (13%)
2	TLA	B	402	-	3,9,9	0.46	0	6,12,12	0.89	0
2	TLA	D	402	4	3,9,9	0.32	0	6,12,12	0.83	0
2	TLA	A	402	4	3,9,9	0.35	0	6,12,12	1.26	1 (16%)
2	TLA	C	403	4	3,9,9	0.55	0	6,12,12	1.29	2 (33%)
2	TLA	D	401	-	3,9,9	0.66	0	6,12,12	0.75	0
2	TLA	B	401	-	3,9,9	0.46	0	6,12,12	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	403	4	-	5/12/32/32	0/3/3/3
2	TLA	B	403	4	-	4/4/12/12	-
2	TLA	C	401	-	-	0/4/12/12	-
2	TLA	A	401	-	-	2/4/12/12	-
3	ADP	A	403	4	-	2/12/32/32	0/3/3/3
3	ADP	C	404	4	-	3/12/32/32	0/3/3/3
2	TLA	C	402	-	-	3/4/12/12	-
3	ADP	B	404	4	-	4/12/32/32	0/3/3/3
2	TLA	B	402	-	-	1/4/12/12	-
2	TLA	D	402	4	-	4/4/12/12	-
2	TLA	A	402	4	-	4/4/12/12	-
2	TLA	C	403	4	-	4/4/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLA	D	401	-	-	0/4/12/12	-
2	TLA	B	401	-	-	1/4/12/12	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	ADP	O4'-C1'	4.32	1.47	1.41
3	C	404	ADP	O4'-C1'	4.32	1.47	1.41
3	A	403	ADP	O4'-C1'	3.97	1.46	1.41
3	B	404	ADP	O4'-C1'	3.94	1.46	1.41
3	B	404	ADP	PB-O1B	3.54	1.62	1.50
3	A	403	ADP	PB-O1B	3.48	1.61	1.50
3	A	403	ADP	C8-N7	-2.37	1.30	1.34
3	C	404	ADP	C8-N7	-2.29	1.30	1.34
3	D	403	ADP	C8-N7	-2.26	1.30	1.34
3	B	404	ADP	C8-N7	-2.01	1.31	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	403	ADP	PA-O3A-PB	-5.77	113.02	132.83
3	C	404	ADP	PA-O3A-PB	-5.44	114.17	132.83
3	A	403	ADP	PA-O3A-PB	-5.31	114.61	132.83
3	B	404	ADP	PA-O3A-PB	-5.24	114.83	132.83
3	C	404	ADP	N3-C2-N1	-4.70	121.34	128.68
3	A	403	ADP	N3-C2-N1	-4.53	121.60	128.68
3	B	404	ADP	N3-C2-N1	-4.47	121.69	128.68
3	D	403	ADP	N3-C2-N1	-4.32	121.92	128.68
2	A	402	TLA	C4-C3-C2	-2.27	108.21	113.11
3	B	404	ADP	PA-O5'-C5'	-2.22	108.64	121.68
2	C	403	TLA	C1-C2-C3	-2.21	108.36	113.11
2	B	403	TLA	C1-C2-C3	-2.17	108.44	113.11
3	D	403	ADP	O3B-PB-O3A	2.16	111.89	104.64
3	B	404	ADP	C4-C5-N7	-2.16	107.15	109.40
3	D	403	ADP	PA-O5'-C5'	-2.12	109.27	121.68
3	C	404	ADP	PA-O5'-C5'	-2.11	109.29	121.68
2	C	403	TLA	C4-C3-C2	-2.06	108.67	113.11
3	D	403	ADP	C4-C5-N7	-2.06	107.25	109.40
3	A	403	ADP	PA-O5'-C5'	-2.06	109.61	121.68
3	A	403	ADP	C4-C5-N7	-2.02	107.30	109.40
2	B	403	TLA	C4-C3-C2	-2.01	108.78	113.11

There are no chirality outliers.

All (37) torsion outliers are listed below:

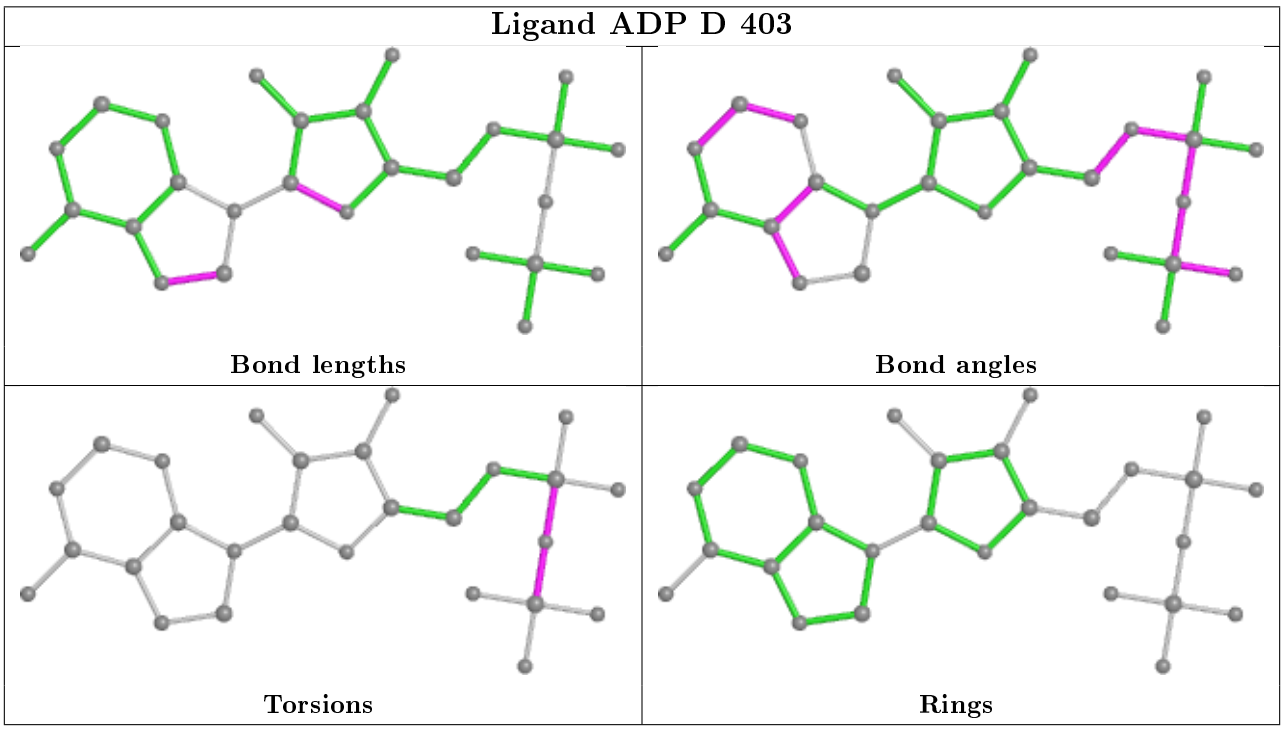
Mol	Chain	Res	Type	Atoms
2	B	403	TLA	C1-C2-C3-O3
2	B	403	TLA	C1-C2-C3-C4
2	B	403	TLA	O2-C2-C3-O3
2	B	403	TLA	O2-C2-C3-C4
2	C	402	TLA	C1-C2-C3-C4
3	D	403	ADP	PA-O3A-PB-O3B
2	A	401	TLA	C1-C2-C3-C4
2	A	402	TLA	C1-C2-C3-C4
2	D	402	TLA	C1-C2-C3-C4
2	C	403	TLA	C1-C2-C3-O3
2	C	403	TLA	C1-C2-C3-C4
2	C	403	TLA	O2-C2-C3-C4
2	A	402	TLA	O2-C2-C3-O3
2	B	401	TLA	C1-C2-C3-C4
2	C	403	TLA	O2-C2-C3-O3
3	B	404	ADP	PB-O3A-PA-O1A
3	D	403	ADP	PB-O3A-PA-O1A
3	A	403	ADP	PB-O3A-PA-O1A
2	A	402	TLA	C1-C2-C3-O3
2	A	402	TLA	O2-C2-C3-C4
3	B	404	ADP	PA-O3A-PB-O1B
3	C	404	ADP	PA-O3A-PB-O2B
3	C	404	ADP	PA-O3A-PB-O3B
3	A	403	ADP	PA-O3A-PB-O3B
3	C	404	ADP	PB-O3A-PA-O1A
3	D	403	ADP	PB-O3A-PA-O2A
2	C	402	TLA	C1-C2-C3-O3
2	C	402	TLA	O2-C2-C3-C4
2	D	402	TLA	C1-C2-C3-O3
2	D	402	TLA	O2-C2-C3-C4
3	D	403	ADP	PA-O3A-PB-O1B
3	B	404	ADP	PA-O3A-PB-O2B
3	B	404	ADP	PA-O3A-PB-O3B
3	D	403	ADP	PA-O3A-PB-O2B
2	B	402	TLA	C1-C2-C3-C4
2	D	402	TLA	O2-C2-C3-O3
2	A	401	TLA	O2-C2-C3-C4

There are no ring outliers.

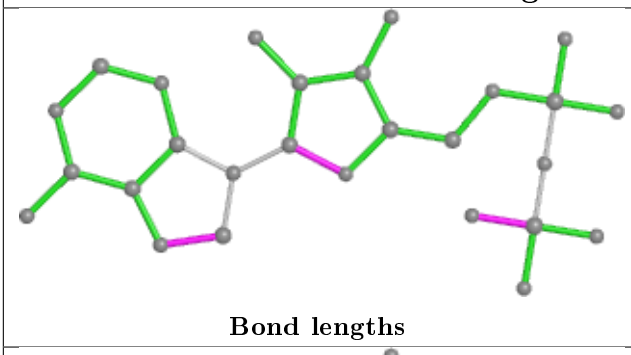
9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	ADP	1	0
2	B	403	TLA	1	0
2	A	401	TLA	1	0
3	A	403	ADP	3	0
3	C	404	ADP	1	0
3	B	404	ADP	2	0
2	B	402	TLA	2	0
2	D	402	TLA	1	0
2	D	401	TLA	2	0

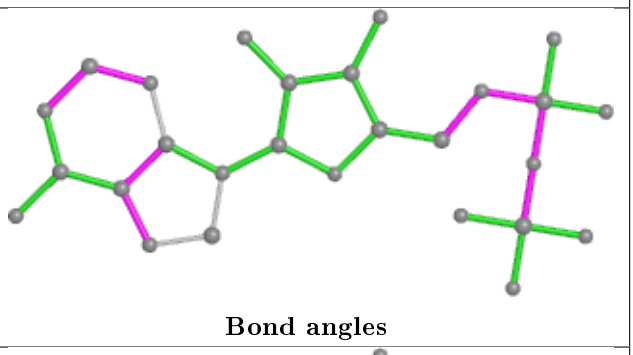
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



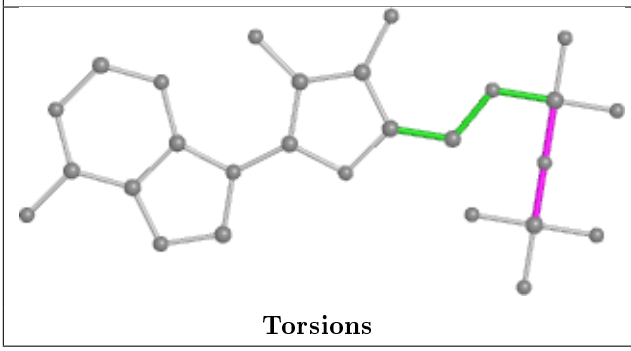
Ligand ADP A 403



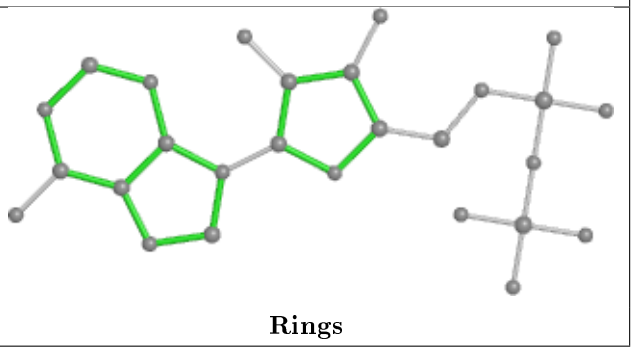
Bond lengths



Bond angles

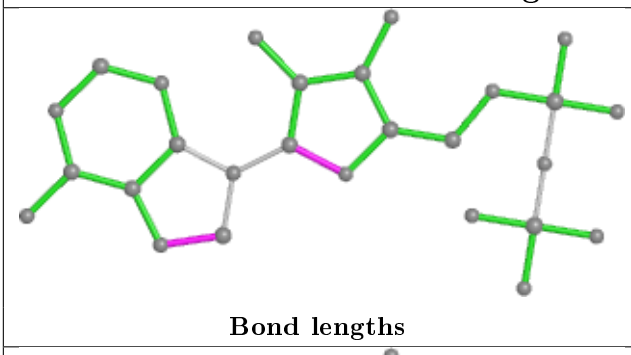


Torsions

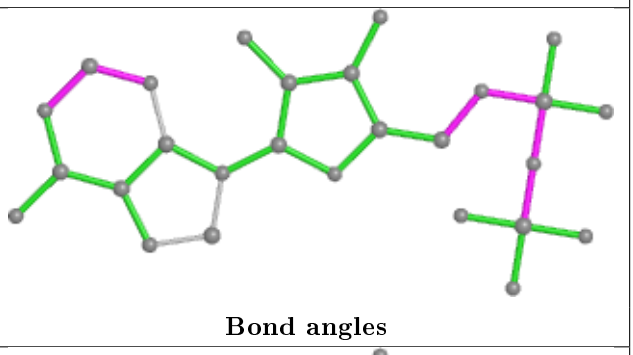


Rings

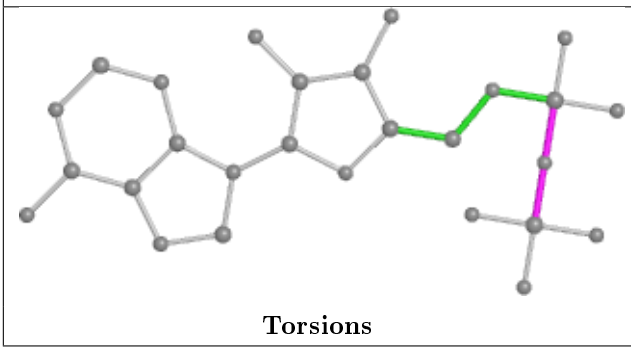
Ligand ADP C 404



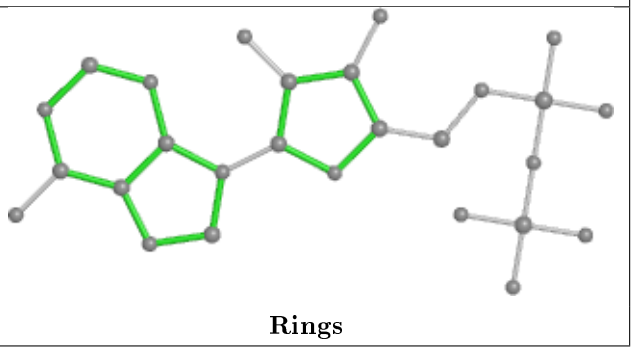
Bond lengths



Bond angles

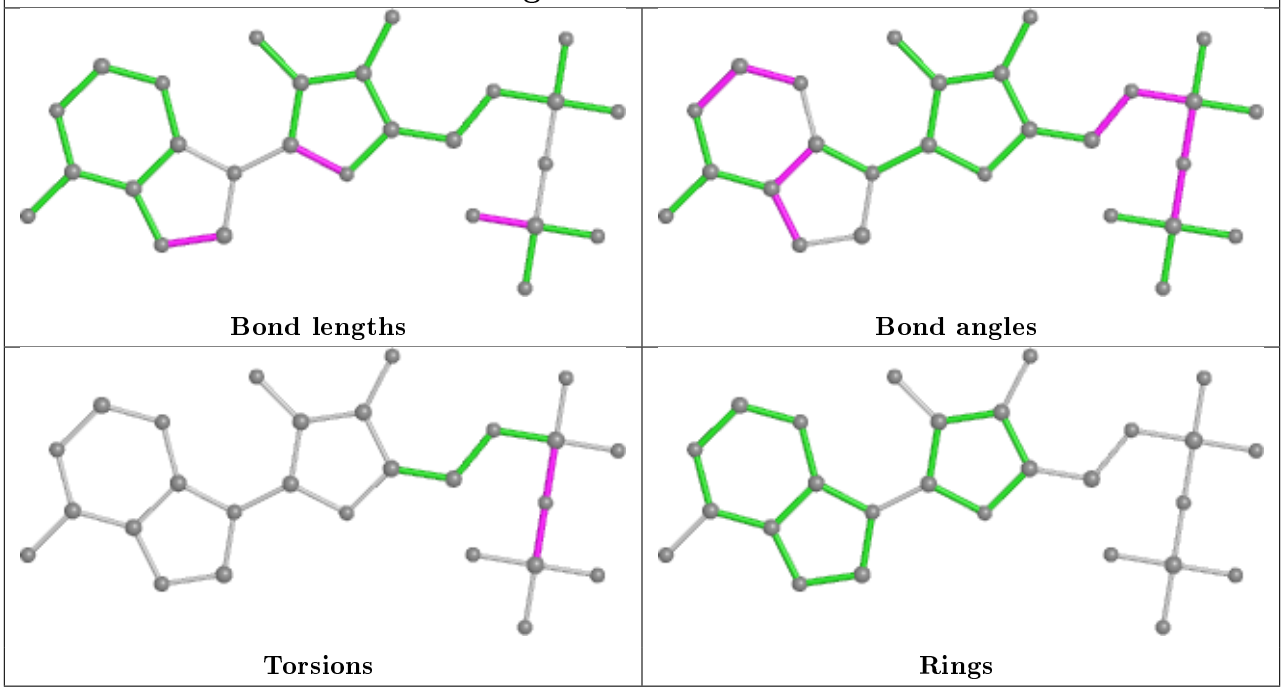


Torsions



Rings

Ligand ADP B 404



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, 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	291/307 (94%)	0.17	11 (3%) 40 47	10, 21, 34, 43	0
1	B	291/307 (94%)	0.01	7 (2%) 59 66	9, 20, 38, 66	0
1	C	291/307 (94%)	0.25	8 (2%) 54 62	15, 25, 40, 55	0
1	D	291/307 (94%)	0.15	9 (3%) 49 56	12, 24, 41, 62	0
All	All	1164/1228 (94%)	0.15	35 (3%) 50 57	9, 23, 39, 66	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	43	VAL	4.8
1	A	2	GLY	4.7
1	D	75	HIS	3.7
1	D	42	THR	3.7
1	B	41	GLY	3.5
1	B	298	LYS	3.3
1	C	209	ASP	3.2
1	D	41	GLY	3.2
1	C	227	GLU	3.2
1	C	132	ARG	3.1
1	D	76	VAL	3.1
1	D	44	ASP	2.9
1	C	228	ASP	2.8
1	A	129	PRO	2.8
1	B	42	THR	2.7
1	A	76	VAL	2.7
1	A	227	GLU	2.6
1	C	247	ASP	2.5
1	C	130	GLU	2.5
1	B	2	GLY	2.4
1	A	228	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	283	GLU	2.4
1	B	3	ILE	2.3
1	A	247	ASP	2.3
1	D	45	TRP	2.2
1	B	76	VAL	2.1
1	B	40	ASP	2.1
1	D	71	GLU	2.1
1	A	126	ALA	2.1
1	A	47	ARG	2.1
1	D	47	ARG	2.1
1	A	261	ALA	2.0
1	A	132	ARG	2.0
1	C	156	GLU	2.0
1	C	2	GLY	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	TLA	C	401	10/10	0.67	0.40	66,69,70,72	0
4	MG	D	405	1/1	0.76	0.16	34,34,34,34	0
2	TLA	C	402	10/10	0.80	0.34	46,48,51,52	0
2	TLA	B	401	10/10	0.80	0.38	60,61,63,63	0
2	TLA	B	402	10/10	0.80	0.41	68,70,71,72	0
2	TLA	D	402	10/10	0.81	0.21	33,42,45,47	0
2	TLA	A	401	10/10	0.85	0.36	48,50,52,53	0
4	MG	C	406	1/1	0.86	0.26	28,28,28,28	0
2	TLA	D	401	10/10	0.87	0.48	55,58,60,61	0

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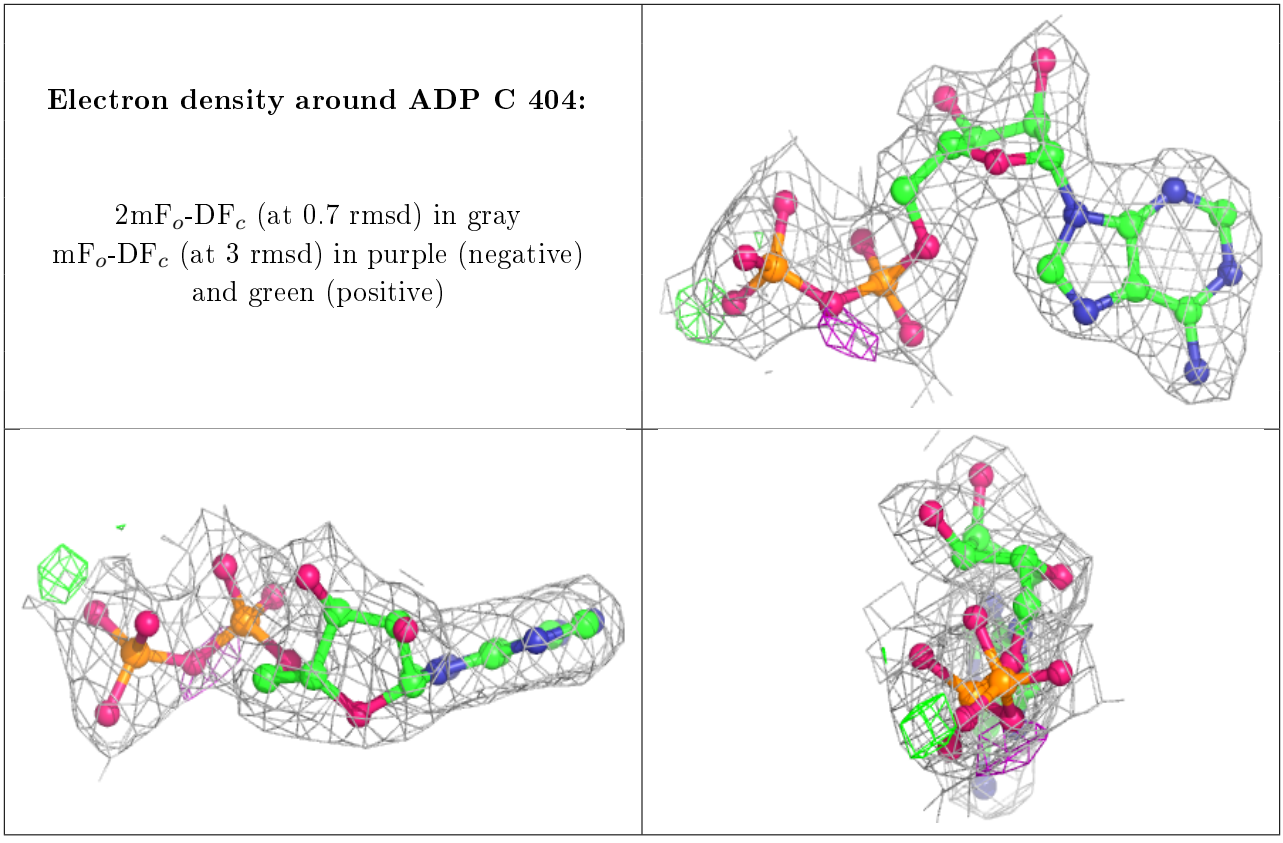
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TLA	C	403	10/10	0.88	0.20	33,37,45,46	0
4	MG	D	406	1/1	0.91	0.16	33,33,33,33	0
4	MG	D	404	1/1	0.93	0.16	22,22,22,22	0
2	TLA	B	403	10/10	0.93	0.14	26,33,36,37	0
2	TLA	A	402	10/10	0.94	0.17	24,28,35,36	0
4	MG	B	406	1/1	0.95	0.12	24,24,24,24	0
4	MG	A	404	1/1	0.96	0.13	22,22,22,22	0
4	MG	C	405	1/1	0.96	0.12	29,29,29,29	0
3	ADP	C	404	27/27	0.96	0.15	19,24,26,27	0
4	MG	A	405	1/1	0.96	0.21	20,20,20,20	0
3	ADP	A	403	27/27	0.97	0.12	14,17,19,21	0
3	ADP	D	403	27/27	0.97	0.12	12,17,19,19	0
4	MG	B	405	1/1	0.98	0.12	19,19,19,19	0
3	ADP	B	404	27/27	0.98	0.10	11,13,16,19	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.

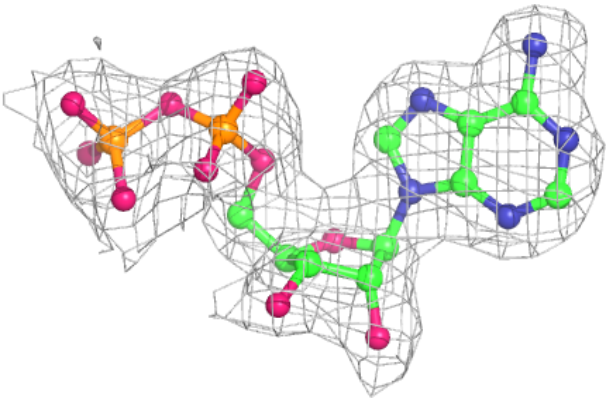
Electron density around ADP C 404:

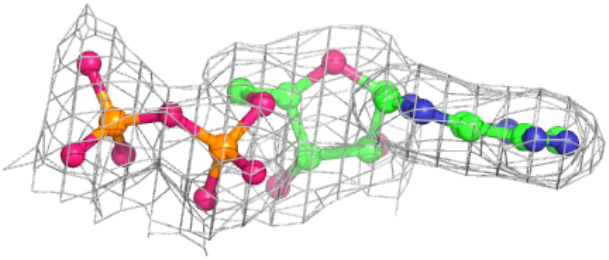
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

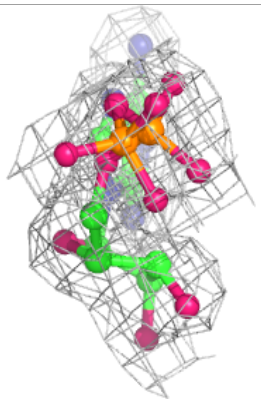


Electron density around ADP A 403:

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

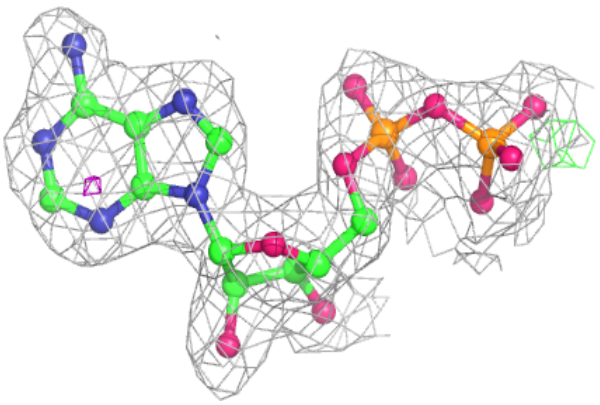


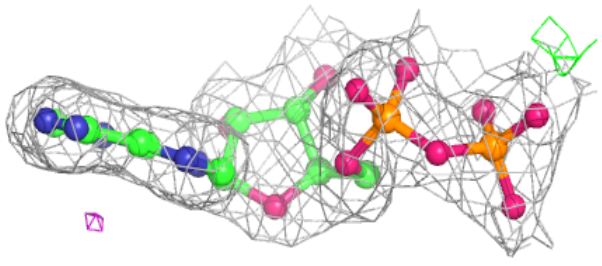


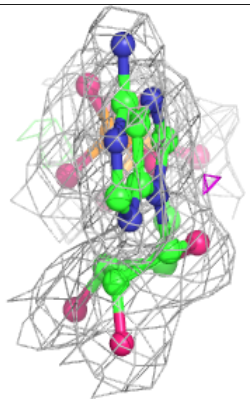


Electron density around ADP D 403:

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

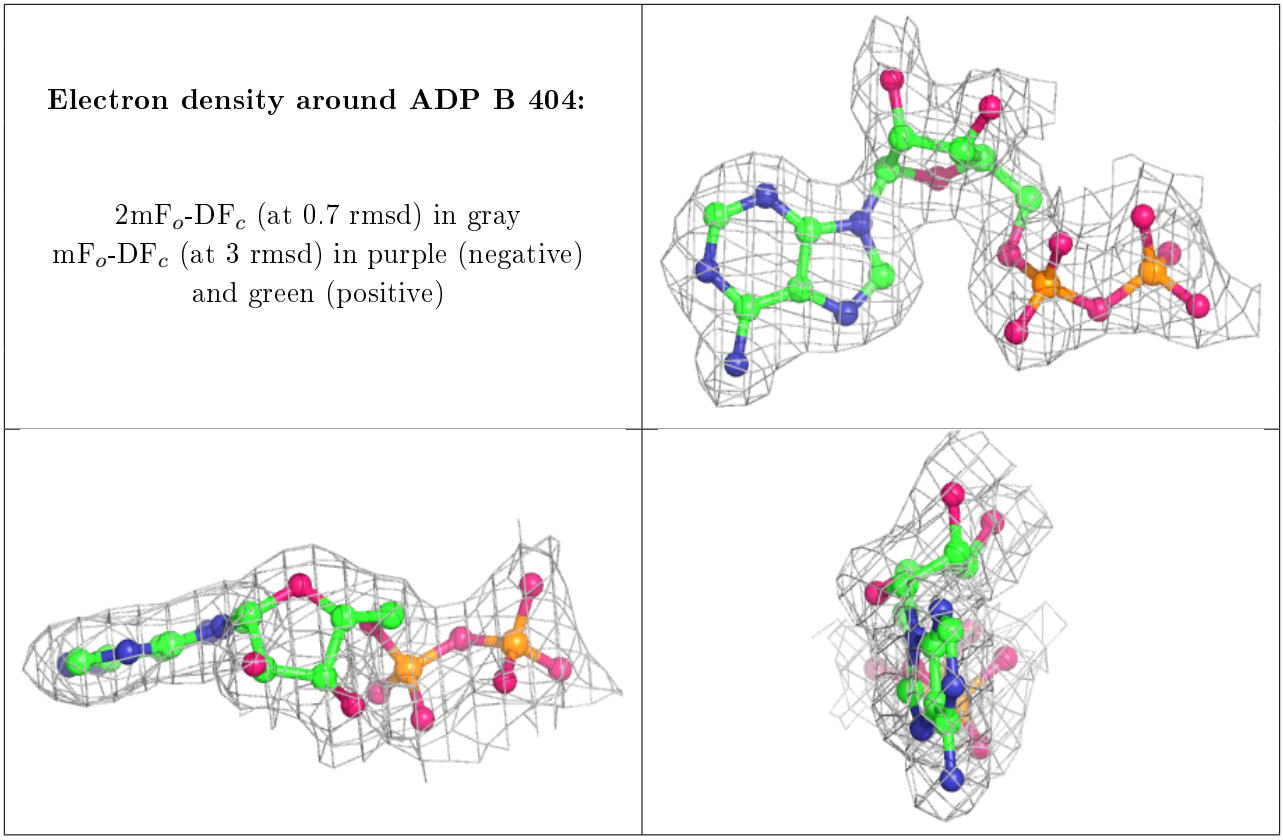






Electron density around ADP B 404:

$2mF_o$-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

There are no such residues in this entry.