Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2024 – 08:04 PM EDT

PDB ID	:	9C10
Title	:	AMG 193, a clinical stage MTA-cooperative PRMT5 inhibitor, drives anti-tumor activity preclinically and in patients with MTAP-deleted cancers
Authors	:	Ghimire-Rijal, S.; Mukund, S.
Deposited on	:	2024-05-28
Resolution	:	2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

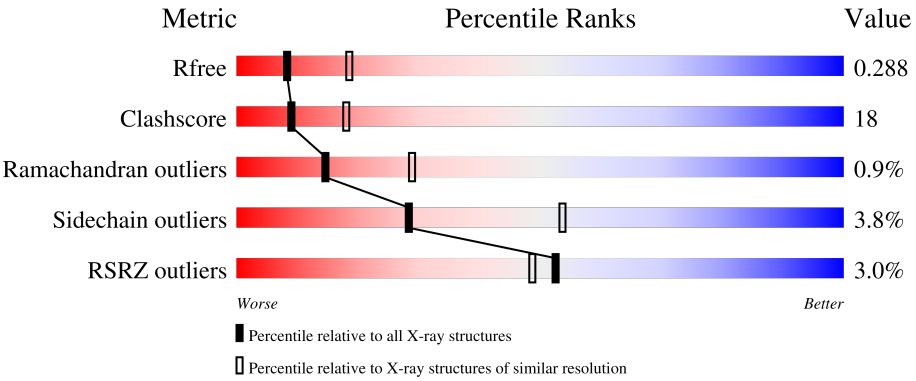
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 2.85 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}	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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	650	2% 68% 25%
2	B	344	5% 61% 27% 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7409 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 Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			4996	3196	851	926	23			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP O14744
A	-11	ASP	-	expression tag	UNP O14744
A	-10	TYR	-	expression tag	UNP O14744
A	-9	LYS	-	expression tag	UNP O14744
A	-8	ASP	-	expression tag	UNP O14744
A	-7	ASP	-	expression tag	UNP O14744
A	-6	ASP	-	expression tag	UNP O14744
A	-5	ASP	-	expression tag	UNP O14744
A	-4	LYS	-	expression tag	UNP O14744
A	-3	GLY	-	expression tag	UNP O14744
A	-2	ARG	-	expression tag	UNP O14744
A	-1	ALA	-	expression tag	UNP O14744
A	0	THR	-	expression tag	UNP O14744

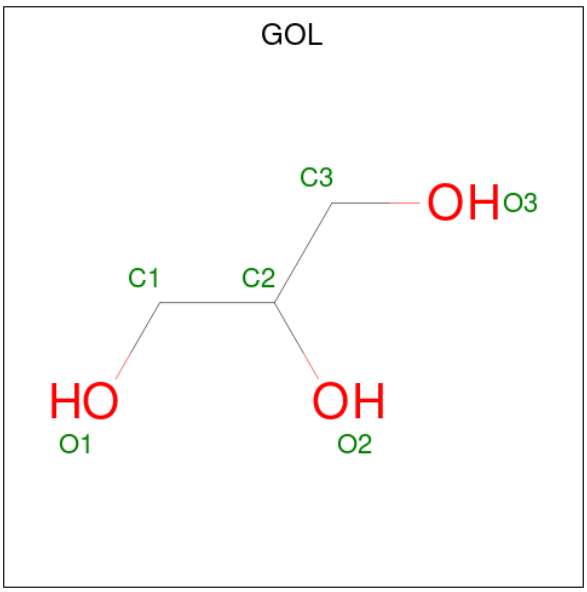
- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	309	Total	C	N	O	S	0	0	0
			2298	1443	390	451	14			

There are 3 discrepancies between the modelled and reference sequences:

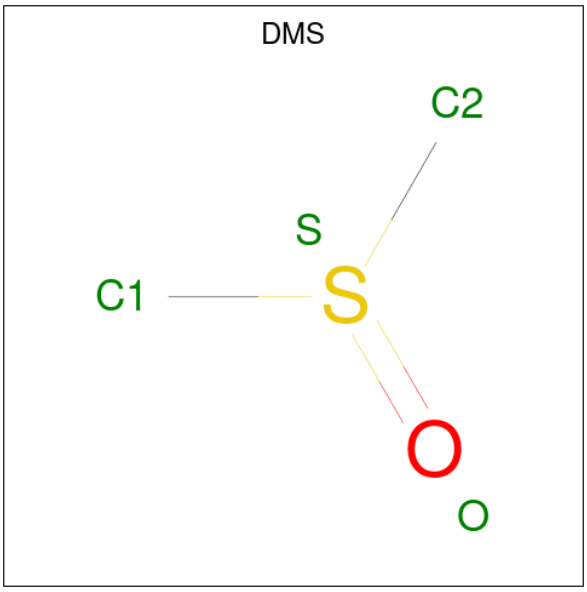
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q9BQA1
B	0	SER	-	expression tag	UNP Q9BQA1
B	1	LEU	-	expression tag	UNP Q9BQA1

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



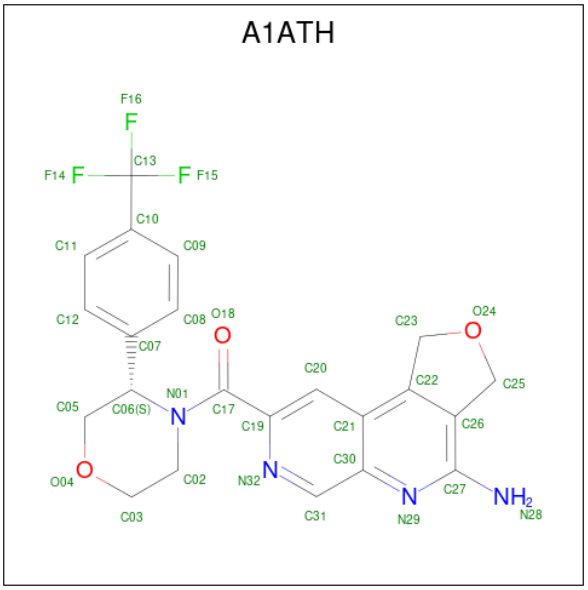
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



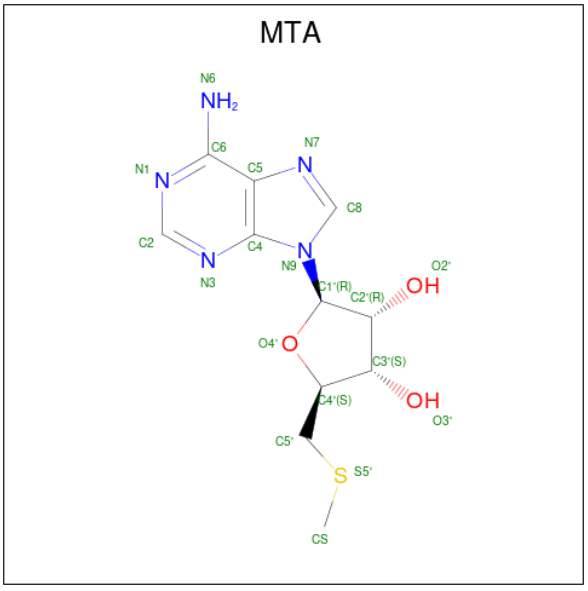
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is (4-amino-1,3-dihydrofuro[3,4-c][1,7]naphthyridin-8-yl){(3S)-3-[4-(trifluoromethyl)phenyl]morpholin-4-yl}methanone (three-letter code: A1ATH) (formula: $C_{22}H_{19}F_3N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
5	A	1	32	22	3	4	3	0	0

- Molecule 6 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA) (formula: $C_{11}H_{15}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 7 is water.

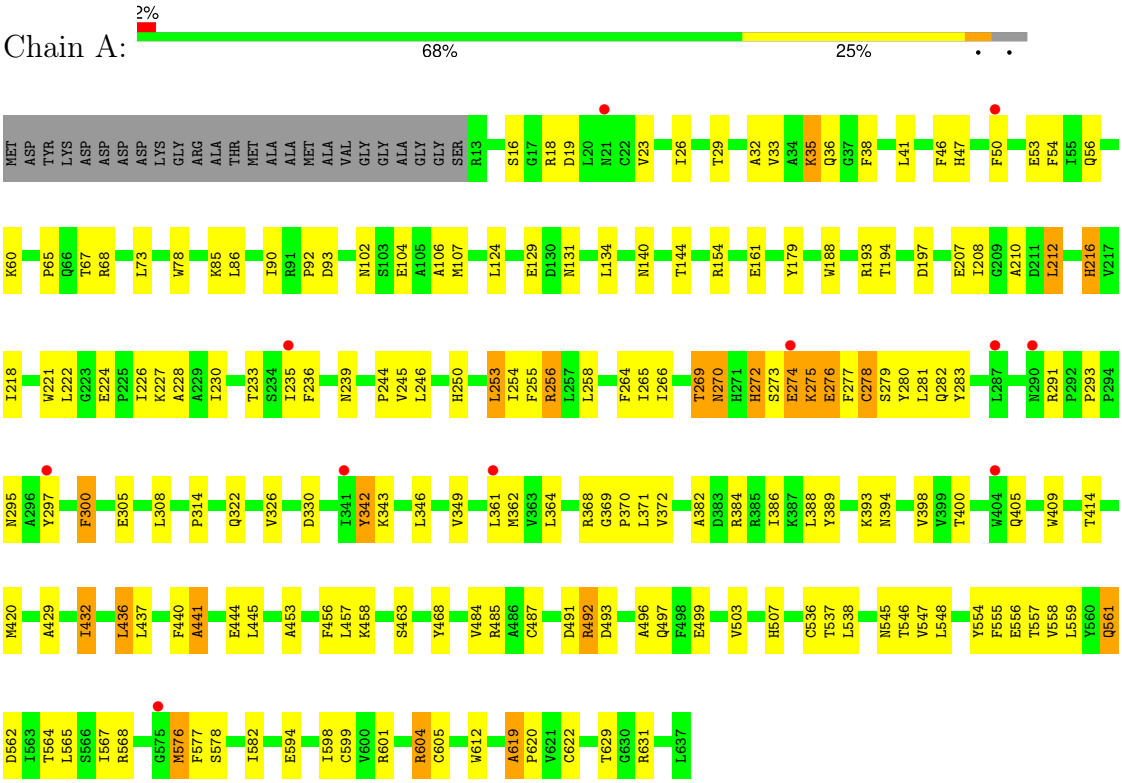
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	42	Total	O	0	0
			42	42		
7	B	5	Total	O	0	0
			5	5		

3 Residue-property plots

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

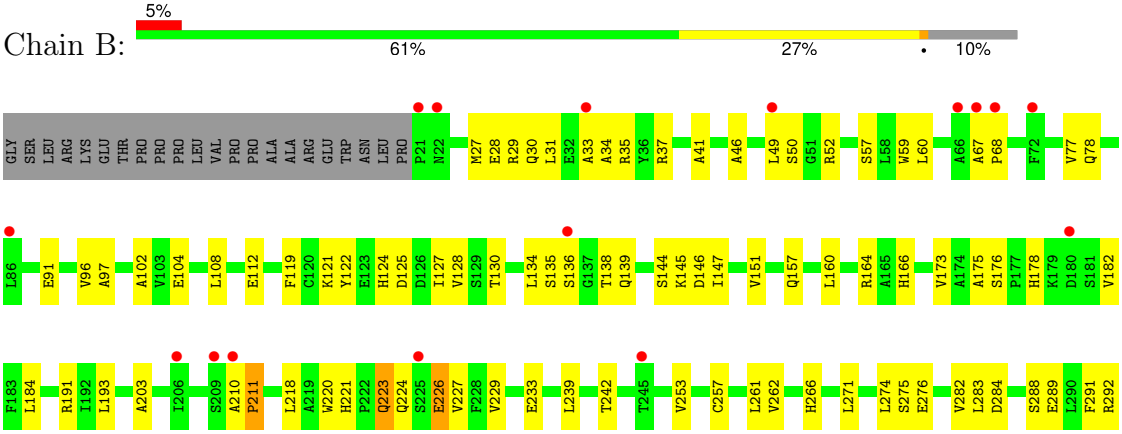
• Molecule 1: Protein arginine N-methyltransferase 5

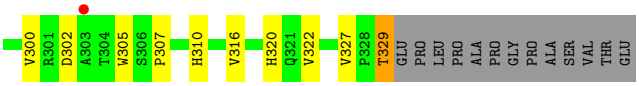
Chain A:



• Molecule 2: Methylosome protein 50

Chain B:




V300
R301
D302
A303
T304
W305
S306
P307
H310
V316
H320
Q321
V322
V327
P328
T329
GLU
PRO
LEU
PRO
ALA
PRO
GLY
PRO
ALA
SER
VAL
THR
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	103.65Å 138.16Å 178.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.32 – 2.85 41.32 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.9 (41.32-2.85) 93.8 (41.32-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.261 , 0.299 0.258 , 0.288	Depositor DCC
R_{free} test set	1514 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7409	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: MTA, A1ATH, GOL, DMS

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	0.39	0/5138	0.55	0/7004
2	B	0.29	0/2354	0.56	0/3222
All	All	0.36	0/7492	0.55	0/10226

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

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	4996	0	4814	173	0
2	B	2298	0	2184	94	0
3	A	12	0	16	1	0
4	A	4	0	6	0	0
5	A	32	0	0	0	0
6	A	20	0	14	2	0
7	A	42	0	0	0	0
7	B	5	0	0	0	0
All	All	7409	0	7034	260	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 18.

All (260) 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)
2:B:221:HIS:HB3	2:B:227:VAL:CG1	1.72	1.18
1:A:619:ALA:HB1	1:A:620:PRO:HD3	1.30	1.14
1:A:619:ALA:CB	1:A:620:PRO:HD3	1.80	1.10
1:A:212:LEU:HD23	1:A:218:ILE:HD11	1.18	1.10
2:B:221:HIS:HE1	2:B:223:GLN:HB2	1.09	1.09
2:B:221:HIS:HB3	2:B:227:VAL:HG13	1.33	1.07
2:B:221:HIS:CE1	2:B:223:GLN:HB2	1.92	1.04
1:A:619:ALA:CB	1:A:620:PRO:CD	2.35	1.03
1:A:604:ARG:HH11	1:A:604:ARG:HG2	1.27	0.99
1:A:212:LEU:CD2	1:A:218:ILE:HD11	1.92	0.98
2:B:221:HIS:CB	2:B:227:VAL:HG13	1.92	0.98
2:B:226:GLU:O	2:B:242:THR:HG22	1.68	0.94
1:A:619:ALA:HB3	1:A:620:PRO:CD	1.97	0.94
1:A:273:SER:C	1:A:275:LYS:H	1.69	0.93
1:A:179:TYR:CE1	1:A:216:HIS:CE1	2.59	0.91
2:B:221:HIS:CB	2:B:227:VAL:CG1	2.47	0.87
1:A:273:SER:C	1:A:275:LYS:N	2.29	0.84
1:A:212:LEU:HD23	1:A:218:ILE:CD1	2.06	0.82
2:B:223:GLN:HA	2:B:223:GLN:NE2	1.98	0.78
1:A:305:GLU:OE2	1:A:507:HIS:CG	2.37	0.77
1:A:179:TYR:CD1	1:A:216:HIS:CE1	2.72	0.77
2:B:57:SER:HG	2:B:59:TRP:HE1	1.32	0.74
2:B:221:HIS:HB3	2:B:227:VAL:HG12	1.70	0.72
1:A:445:LEU:N	1:A:445:LEU:HD23	2.04	0.72
2:B:41:ALA:HB1	2:B:60:LEU:HD11	1.72	0.72
1:A:346:LEU:HD21	1:A:382:ALA:HB1	1.71	0.71
1:A:273:SER:HA	1:A:275:LYS:NZ	2.05	0.71
1:A:278:CYS:O	1:A:282:GLN:N	2.20	0.71
1:A:253:LEU:O	1:A:253:LEU:HD22	1.90	0.71
1:A:274:GLU:O	1:A:275:LYS:O	2.08	0.70
1:A:619:ALA:HB1	1:A:620:PRO:CD	2.10	0.70
1:A:33:VAL:HG21	1:A:41:LEU:HD13	1.73	0.69
1:A:364:LEU:HD23	1:A:420:MET:HE3	1.73	0.69
1:A:254:ILE:HG22	1:A:258:LEU:CD2	2.22	0.69
1:A:239:ASN:HB3	1:A:245:VAL:HG21	1.73	0.69
1:A:179:TYR:CE1	1:A:216:HIS:ND1	2.61	0.68
1:A:50:PHE:HD2	2:B:49:LEU:HB3	1.56	0.68
1:A:619:ALA:HB3	1:A:620:PRO:HD2	1.76	0.68
1:A:604:ARG:HG2	1:A:604:ARG:NH1	2.02	0.68
2:B:67:ALA:HB3	2:B:322:VAL:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:LEU:HD12	2:B:139:GLN:HB2	1.76	0.67
2:B:193:LEU:HD12	2:B:203:ALA:HB1	1.75	0.67
1:A:19:ASP:OD2	1:A:154:ARG:NH1	2.25	0.67
1:A:50:PHE:CD2	2:B:49:LEU:HB3	2.30	0.66
1:A:193:ARG:NH1	1:A:224:GLU:OE1	2.29	0.65
1:A:179:TYR:CZ	1:A:216:HIS:ND1	2.65	0.65
1:A:405:GLN:HA	1:A:409:TRP:HB2	1.78	0.65
1:A:314:PRO:HD2	1:A:444:GLU:HG2	1.78	0.65
1:A:279:SER:HA	1:A:282:GLN:HB2	1.78	0.64
1:A:362:MET:HG2	1:A:389:TYR:HB2	1.79	0.64
1:A:420:MET:HG2	6:A:705:MTA:N1	2.13	0.63
1:A:273:SER:O	1:A:275:LYS:N	2.30	0.63
2:B:329:THR:O	2:B:329:THR:OG1	2.17	0.62
2:B:226:GLU:C	2:B:242:THR:HG22	2.19	0.62
1:A:254:ILE:O	1:A:258:LEU:HD22	2.00	0.62
1:A:255:PHE:HA	1:A:258:LEU:HD23	1.80	0.62
2:B:271:LEU:O	2:B:283:LEU:N	2.30	0.62
1:A:254:ILE:O	1:A:258:LEU:CD2	2.47	0.61
2:B:78:GLN:N	2:B:78:GLN:OE1	2.33	0.61
1:A:305:GLU:OE2	1:A:507:HIS:ND1	2.33	0.61
2:B:221:HIS:HB2	2:B:227:VAL:HG13	1.78	0.61
1:A:558:VAL:HG12	1:A:558:VAL:O	2.00	0.60
1:A:346:LEU:N	1:A:346:LEU:HD23	2.16	0.60
2:B:34:ALA:O	2:B:35:ARG:HD3	2.02	0.60
1:A:38:PHE:CZ	1:A:281:LEU:HD11	2.37	0.60
1:A:537:THR:HG23	1:A:601:ARG:HD3	1.83	0.60
2:B:166:HIS:CE1	2:B:193:LEU:HD23	2.36	0.60
1:A:255:PHE:HE1	1:A:291:ARG:CB	2.15	0.59
1:A:245:VAL:HG12	1:A:246:LEU:H	1.68	0.59
1:A:554:TYR:HB3	1:A:567:ILE:HG13	1.83	0.59
2:B:57:SER:OG	2:B:59:TRP:NE1	2.29	0.59
1:A:276:GLU:HA	1:A:276:GLU:OE1	2.02	0.59
1:A:86:LEU:HD13	1:A:124:LEU:HD21	1.84	0.59
2:B:224:GLN:HB2	2:B:227:VAL:HG12	1.86	0.58
2:B:305:TRP:CZ3	2:B:327:VAL:HG21	2.38	0.58
1:A:104:GLU:OE2	3:A:701:GOL:H11	2.03	0.58
1:A:349:VAL:O	1:A:384:ARG:NH1	2.36	0.58
1:A:47:HIS:HB3	1:A:50:PHE:HB2	1.84	0.58
2:B:29:ARG:HH11	2:B:29:ARG:HG3	1.69	0.58
1:A:300:PHE:N	1:A:300:PHE:CD1	2.72	0.57
1:A:36:GLN:NE2	1:A:277:PHE:HD2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:SER:HA	1:A:275:LYS:HZ3	1.70	0.57
1:A:429:ALA:HB3	1:A:457:LEU:HA	1.84	0.57
2:B:191:ARG:HD2	2:B:193:LEU:HD21	1.86	0.57
1:A:437:LEU:HD21	1:A:468:TYR:CE2	2.40	0.57
2:B:305:TRP:HZ3	2:B:327:VAL:HG21	1.70	0.57
1:A:372:VAL:HG23	1:A:388:LEU:CD2	2.36	0.56
2:B:316:VAL:HG12	2:B:322:VAL:HG12	1.86	0.56
1:A:254:ILE:HG22	1:A:258:LEU:HD21	1.87	0.56
1:A:300:PHE:HD1	1:A:300:PHE:H	1.53	0.56
2:B:128:VAL:HA	2:B:144:SER:HB2	1.87	0.56
1:A:86:LEU:HD21	1:A:90:ILE:HB	1.87	0.56
1:A:212:LEU:HD13	1:A:250:HIS:CD2	2.41	0.55
2:B:223:GLN:HA	2:B:223:GLN:HE21	1.72	0.55
1:A:244:PRO:HD3	1:A:272:HIS:CD2	2.41	0.55
2:B:97:ALA:HB1	2:B:128:VAL:HG12	1.89	0.55
2:B:28:GLU:N	2:B:28:GLU:OE2	2.40	0.55
1:A:369:GLY:N	1:A:370:PRO:HD3	2.21	0.55
1:A:599:CYS:H	1:A:619:ALA:HB2	1.72	0.54
1:A:210:ALA:HA	1:A:235:ILE:HG22	1.90	0.54
2:B:52:ARG:HG2	2:B:52:ARG:HH11	1.72	0.54
1:A:445:LEU:HD23	1:A:445:LEU:H	1.71	0.54
1:A:437:LEU:HD21	1:A:468:TYR:CD2	2.42	0.54
1:A:23:VAL:HG22	1:A:29:THR:HG21	1.90	0.54
2:B:77:VAL:HG22	2:B:78:GLN:H	1.73	0.53
1:A:54:PHE:HE2	1:A:106:ALA:HB2	1.73	0.53
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.89	0.53
2:B:33:ALA:HA	2:B:302:ASP:HB2	1.88	0.53
1:A:221:TRP:HB3	1:A:226:ILE:HD11	1.90	0.53
2:B:68:PRO:HD3	2:B:322:VAL:HG22	1.89	0.53
1:A:273:SER:HA	1:A:275:LYS:HZ2	1.72	0.53
2:B:327:VAL:HG12	2:B:327:VAL:O	2.07	0.53
1:A:207:GLU:HA	1:A:230:ILE:HB	1.89	0.53
1:A:53:GLU:HA	1:A:102:ASN:HD21	1.73	0.52
1:A:228:ALA:HB1	1:A:265:ILE:HD13	1.91	0.52
1:A:436:LEU:CD1	1:A:436:LEU:N	2.73	0.52
2:B:119:PHE:HD2	2:B:121:LYS:HG2	1.75	0.52
1:A:557:THR:HG22	1:A:565:LEU:HB2	1.91	0.52
1:A:18:ARG:NH1	1:A:266:ILE:O	2.43	0.51
1:A:484:VAL:O	1:A:487:CYS:HB2	2.10	0.51
1:A:19:ASP:OD1	1:A:85:LYS:NZ	2.42	0.51
1:A:274:GLU:O	1:A:275:LYS:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:GLU:CA	2:B:242:THR:HG22	2.41	0.51
1:A:86:LEU:HD11	1:A:107:MET:HG3	1.92	0.51
1:A:372:VAL:HG23	1:A:388:LEU:HD22	1.93	0.51
1:A:54:PHE:CE2	1:A:106:ALA:HB2	2.46	0.51
1:A:300:PHE:N	1:A:300:PHE:HD1	2.08	0.51
2:B:223:GLN:NE2	2:B:223:GLN:CA	2.73	0.50
1:A:429:ALA:O	1:A:458:LYS:HG2	2.11	0.50
1:A:233:THR:OG1	1:A:269:THR:O	2.20	0.50
2:B:121:LYS:HE3	2:B:157:GLN:HG3	1.91	0.50
1:A:53:GLU:HA	1:A:102:ASN:ND2	2.27	0.50
1:A:440:PHE:HB2	1:A:582:ILE:HG21	1.93	0.50
2:B:282:VAL:HG22	2:B:291:PHE:HB3	1.94	0.49
1:A:604:ARG:NH1	1:A:604:ARG:CG	2.73	0.49
1:A:322:GLN:O	1:A:326:VAL:HG13	2.12	0.49
2:B:29:ARG:HA	2:B:320:HIS:CD2	2.47	0.49
2:B:262:VAL:HG13	2:B:305:TRP:HE1	1.78	0.49
2:B:274:LEU:HB2	2:B:300:VAL:CG2	2.43	0.49
1:A:270:ASN:HD21	1:A:275:LYS:HA	1.78	0.49
1:A:65:PRO:O	2:B:50:SER:OG	2.24	0.49
1:A:364:LEU:N	1:A:364:LEU:CD1	2.74	0.49
1:A:420:MET:HG2	6:A:705:MTA:C6	2.42	0.48
2:B:102:ALA:HB2	2:B:122:TYR:CD2	2.48	0.48
2:B:284:ASP:OD1	2:B:288:SER:N	2.46	0.48
2:B:146:ASP:O	2:B:164:ARG:NH2	2.47	0.48
2:B:184:LEU:HG	2:B:220:TRP:CZ2	2.48	0.48
1:A:208:ILE:HD12	1:A:253:LEU:CD1	2.44	0.48
1:A:275:LYS:HB3	1:A:276:GLU:H	1.57	0.47
2:B:229:VAL:HG23	2:B:261:LEU:HD13	1.96	0.47
1:A:36:GLN:HE21	1:A:277:PHE:HB2	1.79	0.47
2:B:130:THR:HG23	2:B:173:VAL:HG22	1.97	0.47
2:B:135:SER:OG	2:B:178:HIS:N	2.48	0.47
1:A:254:ILE:O	1:A:258:LEU:HD23	2.14	0.47
1:A:556:GLU:OE1	1:A:568:ARG:HD3	2.14	0.47
1:A:557:THR:CG2	1:A:565:LEU:HB2	2.43	0.47
2:B:29:ARG:HG3	2:B:29:ARG:NH1	2.28	0.47
2:B:29:ARG:HB3	2:B:30:GLN:NE2	2.30	0.47
1:A:245:VAL:HG12	1:A:246:LEU:N	2.28	0.47
1:A:394:ASN:O	1:A:398:VAL:HG23	2.15	0.47
2:B:229:VAL:HG12	2:B:239:LEU:CB	2.45	0.47
1:A:16:SER:HA	1:A:264:PHE:O	2.15	0.47
2:B:266:HIS:NE2	2:B:310:HIS:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:THR:CG2	2:B:124:HIS:O	2.63	0.47
1:A:32:ALA:O	1:A:35:LYS:HG3	2.15	0.47
1:A:140:ASN:O	1:A:144:THR:HG23	2.15	0.46
1:A:197:ASP:CG	1:A:485:ARG:HH22	2.18	0.46
2:B:27:MET:HB3	2:B:59:TRP:CZ2	2.50	0.46
1:A:305:GLU:OE2	1:A:507:HIS:CE1	2.69	0.46
1:A:432:ILE:HD13	1:A:457:LEU:HD13	1.96	0.46
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.73	0.46
1:A:432:ILE:HD11	1:A:463:SER:HB2	1.97	0.46
1:A:436:LEU:N	1:A:436:LEU:HD13	2.29	0.46
2:B:275:SER:OG	2:B:276:GLU:N	2.48	0.46
1:A:330:ASP:OD2	1:A:576:MET:HG2	2.16	0.46
1:A:361:LEU:HD13	1:A:386:ILE:HB	1.98	0.46
2:B:127:ILE:HD12	2:B:145:LYS:HD2	1.98	0.46
1:A:161:GLU:OE1	2:B:191:ARG:NH2	2.48	0.46
1:A:236:PHE:CD2	1:A:280:TYR:CE2	3.04	0.46
1:A:270:ASN:HB3	1:A:277:PHE:CE1	2.51	0.45
1:A:548:LEU:HD22	1:A:598:ILE:HD13	1.99	0.45
1:A:349:VAL:HG13	1:A:384:ARG:HH11	1.81	0.45
2:B:124:HIS:CD2	2:B:128:VAL:HG22	2.50	0.45
2:B:96:VAL:N	2:B:104:GLU:O	2.42	0.45
2:B:157:GLN:O	2:B:157:GLN:HG2	2.16	0.45
1:A:253:LEU:HD22	1:A:253:LEU:C	2.36	0.45
1:A:207:GLU:HG3	1:A:230:ILE:HB	1.99	0.45
1:A:212:LEU:CD2	1:A:218:ILE:CD1	2.80	0.45
1:A:244:PRO:HD3	1:A:272:HIS:HD2	1.82	0.45
1:A:193:ARG:HG3	1:A:194:THR:N	2.31	0.45
1:A:546:THR:OG1	1:A:547:VAL:N	2.50	0.45
2:B:31:LEU:HD23	2:B:46:ALA:HB2	1.98	0.45
1:A:236:PHE:CD2	1:A:280:TYR:HE2	2.35	0.45
1:A:432:ILE:HG23	1:A:457:LEU:HD13	1.98	0.45
1:A:559:LEU:HD21	1:A:565:LEU:HD12	1.98	0.45
2:B:108:LEU:HD12	2:B:112:GLU:HA	1.99	0.44
2:B:227:VAL:HG13	2:B:227:VAL:O	2.17	0.44
2:B:289:GLU:CB	2:B:292:ARG:HH22	2.30	0.44
1:A:389:TYR:CD1	1:A:414:THR:HB	2.53	0.44
1:A:60:LYS:HE2	1:A:60:LYS:HB3	1.68	0.44
1:A:86:LEU:HD13	1:A:124:LEU:CD2	2.48	0.44
1:A:561:GLN:HB3	1:A:562:ASP:H	1.46	0.44
2:B:253:VAL:HG21	2:B:283:LEU:HD11	1.99	0.44
2:B:274:LEU:HB2	2:B:300:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:CD1	1:A:342:TYR:C	2.88	0.44
1:A:493:ASP:HB3	1:A:496:ALA:HB2	1.99	0.44
2:B:37:ARG:NH1	2:B:91:GLU:O	2.44	0.44
2:B:151:VAL:O	2:B:160:LEU:N	2.43	0.44
1:A:222:LEU:HD11	1:A:256:ARG:NH2	2.33	0.43
1:A:536:CYS:SG	1:A:538:LEU:HD21	2.58	0.43
1:A:73:LEU:HB2	1:A:78:TRP:CE2	2.54	0.43
1:A:276:GLU:HB3	1:A:278:CYS:SG	2.58	0.43
2:B:121:LYS:HA	2:B:121:LYS:HD3	1.89	0.43
2:B:136:SER:HB2	2:B:138:THR:HG22	2.00	0.43
1:A:499:GLU:OE2	1:A:631:ARG:NH2	2.48	0.43
2:B:176:SER:HB2	2:B:182:VAL:HG12	1.99	0.43
2:B:224:GLN:HB2	2:B:227:VAL:CG1	2.48	0.43
1:A:86:LEU:CD1	1:A:107:MET:HG3	2.48	0.43
1:A:269:THR:HG21	2:B:124:HIS:O	2.18	0.43
1:A:599:CYS:N	1:A:619:ALA:HB2	2.33	0.43
2:B:96:VAL:HB	2:B:104:GLU:HB2	2.01	0.43
2:B:134:LEU:HD23	2:B:175:ALA:HB1	1.99	0.43
1:A:26:ILE:HD11	1:A:68:ARG:HD3	2.00	0.43
1:A:432:ILE:CD1	1:A:457:LEU:HD22	2.48	0.43
1:A:558:VAL:HG22	1:A:564:THR:HG22	2.01	0.43
2:B:30:GLN:OE1	2:B:49:LEU:N	2.40	0.43
2:B:229:VAL:HG12	2:B:239:LEU:HB3	2.00	0.43
1:A:227:LYS:HD3	1:A:227:LYS:HA	1.77	0.43
1:A:388:LEU:HD23	1:A:389:TYR:N	2.33	0.43
1:A:270:ASN:ND2	1:A:272:HIS:HB2	2.34	0.42
1:A:269:THR:HG22	2:B:125:ASP:HA	2.02	0.42
2:B:233:GLU:HA	2:B:257:CYS:HA	2.00	0.42
2:B:275:SER:O	2:B:300:VAL:HG22	2.19	0.42
1:A:605:CYS:HB2	1:A:612:TRP:CE2	2.54	0.42
2:B:184:LEU:HB3	2:B:218:LEU:HD13	2.01	0.42
1:A:36:GLN:NE2	1:A:277:PHE:CD2	2.86	0.42
1:A:453:ALA:HB1	1:A:456:PHE:CZ	2.55	0.42
1:A:53:GLU:HG2	1:A:56:GLN:HB3	2.02	0.42
1:A:545:ASN:OD1	1:A:594:GLU:N	2.51	0.42
1:A:46:PHE:CD2	1:A:67:THR:HB	2.55	0.42
1:A:92:PRO:HG2	1:A:134:LEU:HD12	2.01	0.42
1:A:629:THR:HG22	1:A:629:THR:O	2.19	0.42
1:A:538:LEU:O	1:A:599:CYS:HA	2.20	0.41
2:B:37:ARG:O	2:B:307:PRO:HG3	2.19	0.41
2:B:210:ALA:HB3	2:B:211:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:ASP:N	2:B:146:ASP:OD1	2.50	0.41
1:A:492:ARG:HG3	1:A:493:ASP:N	2.34	0.41
2:B:52:ARG:HG2	2:B:52:ARG:NH1	2.35	0.41
2:B:68:PRO:HD3	2:B:322:VAL:CG2	2.49	0.41
1:A:197:ASP:O	1:A:485:ARG:NH2	2.54	0.41
1:A:129:GLU:HA	1:A:188:TRP:CD1	2.56	0.41
1:A:93:ASP:OD2	1:A:131:ASN:HA	2.21	0.41
1:A:484:VAL:O	1:A:497:GLN:HG3	2.20	0.41
1:A:429:ALA:HB3	1:A:457:LEU:HD12	2.02	0.41
1:A:368:ARG:HB3	1:A:400:THR:HG21	2.02	0.41
2:B:226:GLU:CA	2:B:242:THR:CG2	2.99	0.41
1:A:246:LEU:HB2	1:A:283:TYR:HE2	1.85	0.40
1:A:272:HIS:O	1:A:275:LYS:HA	2.22	0.40
1:A:38:PHE:CE1	1:A:281:LEU:HD11	2.55	0.40
1:A:432:ILE:H	1:A:432:ILE:HG12	1.73	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	623/650 (96%)	588 (94%)	29 (5%)	6 (1%)	13	26
2	B	307/344 (89%)	285 (93%)	20 (6%)	2 (1%)	19	36
All	All	930/994 (94%)	873 (94%)	49 (5%)	8 (1%)	14	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	LYS
1	A	619	ALA
2	B	147	ILE

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Mol	Chain	Res	Type
1	A	274	GLU
1	A	293	PRO
1	A	441	ALA
1	A	276	GLU
2	B	211	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	543/573 (95%)	516 (95%)	27 (5%)	20 40
2	B	253/291 (87%)	250 (99%)	3 (1%)	67 84
All	All	796/864 (92%)	766 (96%)	30 (4%)	28 54

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

Mol	Chain	Res	Type
1	A	35	LYS
1	A	212	LEU
1	A	216	HIS
1	A	253	LEU
1	A	256	ARG
1	A	269	THR
1	A	270	ASN
1	A	272	HIS
1	A	278	CYS
1	A	295	ASN
1	A	297	TYR
1	A	300	PHE
1	A	342	TYR
1	A	343	LYS
1	A	371	LEU
1	A	393	LYS
1	A	432	ILE
1	A	436	LEU

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Mol	Chain	Res	Type
1	A	491	ASP
1	A	492	ARG
1	A	503	VAL
1	A	561	GLN
1	A	576	MET
1	A	577	PHE
1	A	578	SER
1	A	604	ARG
1	A	622	CYS
2	B	223	GLN
2	B	226	GLU
2	B	329	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	102	ASN
1	A	270	ASN
2	B	169	GLN
2	B	223	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
5	A1ATH	A	704	-	35,36,36	2.11	9 (25%)	49,54,54	1.78	6 (12%)
4	DMS	A	703	-	3,3,3	0.67	0	3,3,3	0.53	0
3	GOL	A	701	-	5,5,5	1.08	0	5,5,5	1.06	0
6	MTA	A	705	-	18,22,22	2.47	4 (22%)	18,32,32	1.70	2 (11%)
3	GOL	A	702	-	5,5,5	0.90	0	5,5,5	1.09	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
5	A1ATH	A	704	-	-	3/18/35/35	0/5/5/5
3	GOL	A	702	-	-	4/4/4/4	-
3	GOL	A	701	-	-	3/4/4/4	-
6	MTA	A	705	-	-	1/3/23/23	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	705	MTA	C1'-N9	-7.96	1.30	1.49
5	A	704	A1ATH	C26-C22	-5.45	1.30	1.37
5	A	704	A1ATH	C21-C30	-5.31	1.34	1.42
5	A	704	A1ATH	C07-C06	4.65	1.58	1.51
5	A	704	A1ATH	C27-N28	4.30	1.45	1.34
6	A	705	MTA	O2'-C2'	-3.78	1.33	1.43
6	A	705	MTA	C6-N6	3.57	1.46	1.34
5	A	704	A1ATH	C06-N01	-3.45	1.44	1.47
5	A	704	A1ATH	C05-C06	-3.37	1.46	1.52
5	A	704	A1ATH	C17-N01	2.79	1.41	1.34
6	A	705	MTA	O3'-C3'	2.76	1.49	1.43
5	A	704	A1ATH	C30-N29	-2.30	1.34	1.37
5	A	704	A1ATH	O18-C17	-2.25	1.17	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	704	A1ATH	C31-N32-C19	8.03	123.75	117.55
6	A	705	MTA	N3-C2-N1	-5.30	121.48	128.67
5	A	704	A1ATH	C20-C19-N32	-4.15	118.37	123.28
5	A	704	A1ATH	C25-O24-C23	-3.07	106.73	110.93
5	A	704	A1ATH	O18-C17-N01	-2.82	117.09	121.62
5	A	704	A1ATH	C03-O04-C05	2.34	113.29	110.02
6	A	705	MTA	C4-C5-N7	-2.32	106.88	109.34
5	A	704	A1ATH	C07-C06-N01	2.30	115.36	111.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	GOL	C1-C2-C3-O3
3	A	702	GOL	O1-C1-C2-C3
3	A	702	GOL	C1-C2-C3-O3
3	A	701	GOL	O2-C2-C3-O3
3	A	702	GOL	O1-C1-C2-O2
3	A	702	GOL	O2-C2-C3-O3
3	A	701	GOL	O1-C1-C2-O2
6	A	705	MTA	O4'-C4'-C5'-S5'
5	A	704	A1ATH	C05-C06-C07-C12
5	A	704	A1ATH	C05-C06-C07-C08
5	A	704	A1ATH	O18-C17-C19-C20

There are no ring outliers.

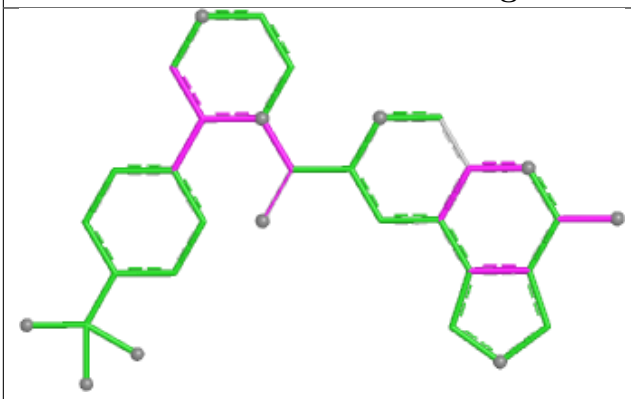
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	GOL	1	0
6	A	705	MTA	2	0

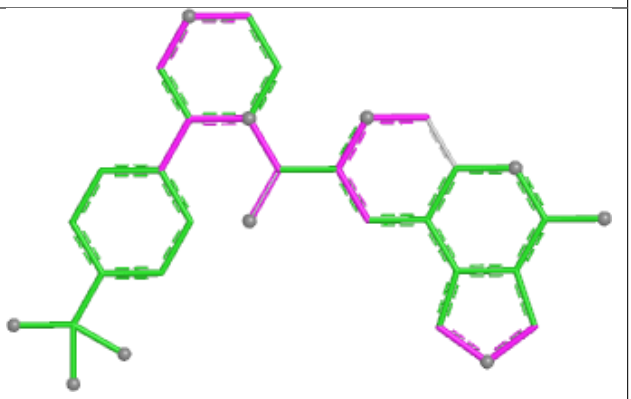
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

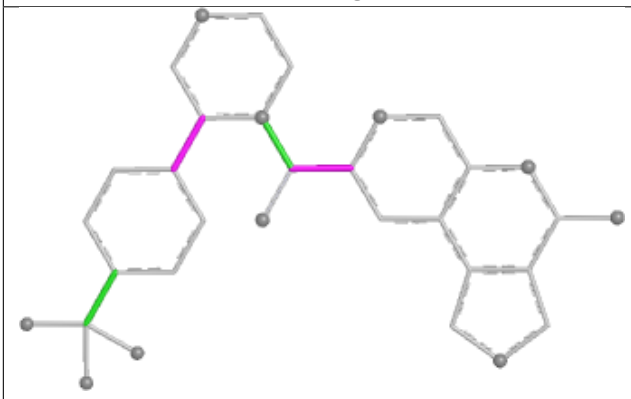
Ligand A1ATH A 704



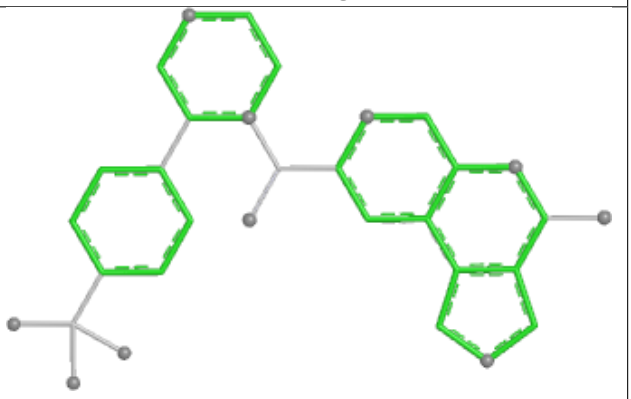
Bond lengths



Bond angles

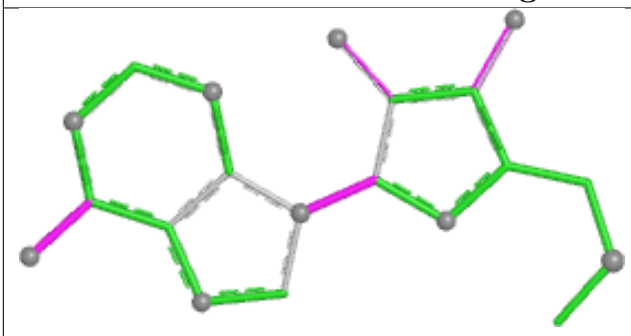


Torsions

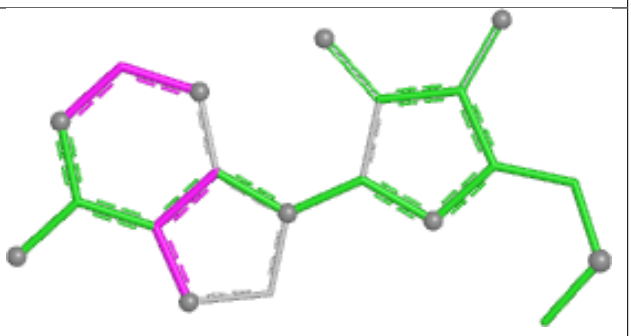


Rings

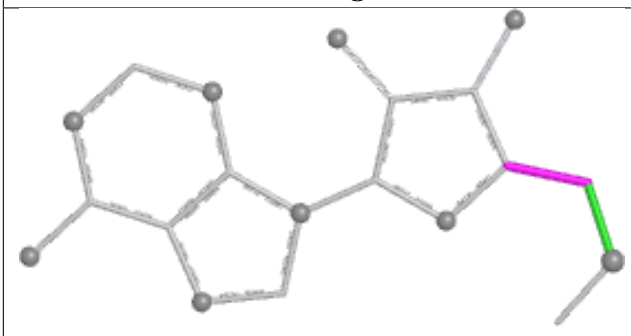
Ligand MTA A 705



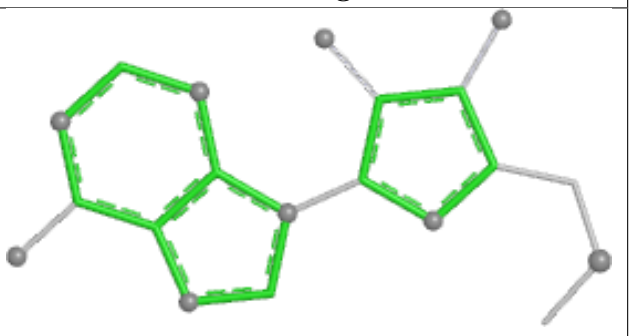
Bond lengths



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	625/650 (96%)	0.33	11 (1%)	67	64	30, 72, 110, 151	0
2	B	309/344 (89%)	0.66	17 (5%)	32	27	69, 90, 116, 148	0
All	All	934/994 (93%)	0.44	28 (2%)	52	49	30, 79, 114, 151	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	225	SER	3.9
2	B	21	PRO	3.7
1	A	297	TYR	3.7
1	A	290	ASN	3.6
2	B	210	ALA	3.2
1	A	50	PHE	3.1
2	B	245	THR	3.1
2	B	180	ASP	2.9
2	B	209	SER	2.8
2	B	86	LEU	2.8
1	A	274	GLU	2.7
2	B	33	ALA	2.7
2	B	206	ILE	2.6
2	B	22	ASN	2.5
1	A	361	LEU	2.5
1	A	404	TRP	2.5
2	B	68	PRO	2.5
2	B	49	LEU	2.5
2	B	72	PHE	2.5
1	A	235	ILE	2.3
2	B	66	ALA	2.3
1	A	575	GLY	2.2
1	A	21	ASN	2.2
2	B	136	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	287	LEU	2.1
2	B	67	ALA	2.1
1	A	341	ILE	2.1
2	B	303	ALA	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)

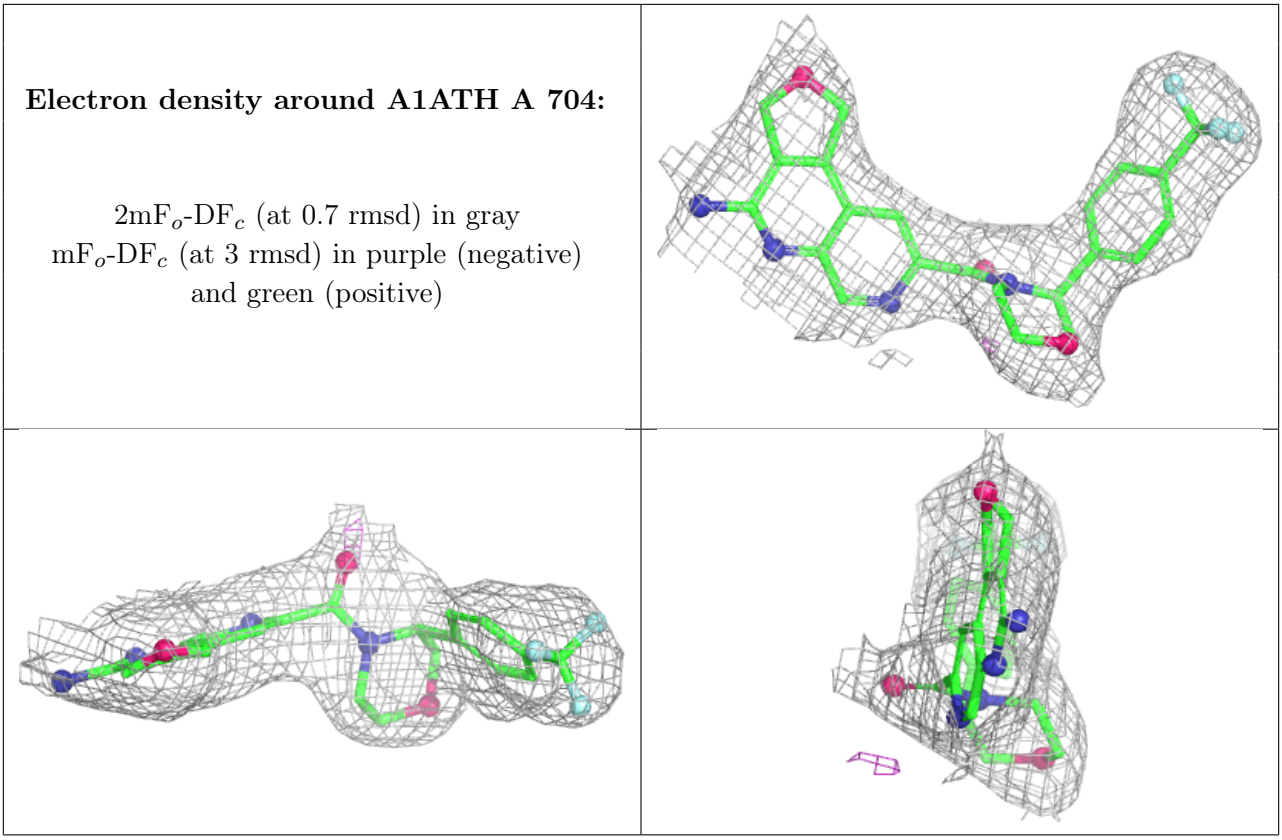
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	GOL	A	701	6/6	0.64	0.16	69,76,81,82	0
4	DMS	A	703	4/4	0.73	0.20	79,88,95,101	0
3	GOL	A	702	6/6	0.83	0.15	66,76,78,79	0
5	A1ATH	A	704	32/32	0.89	0.11	56,63,83,91	0
6	MTA	A	705	20/20	0.92	0.10	59,66,71,75	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.

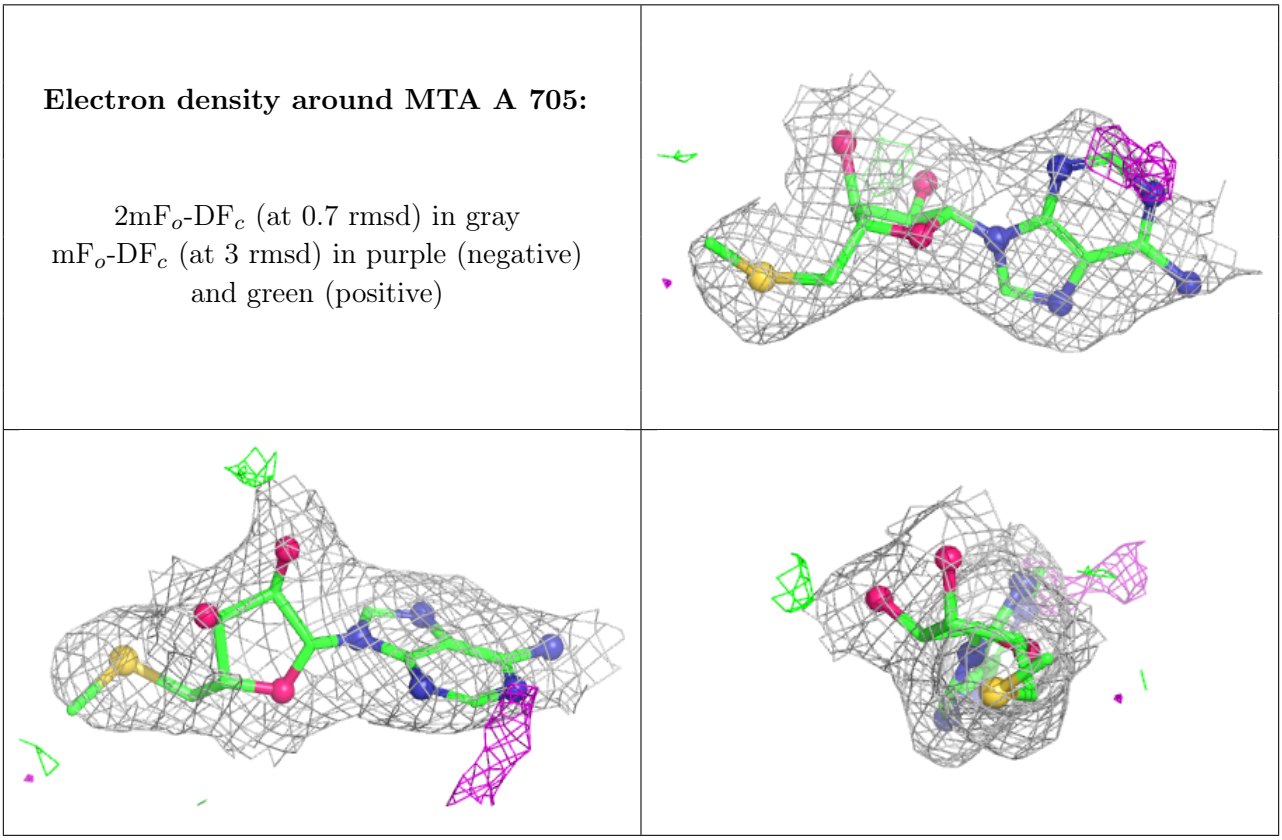
Electron density around A1ATH A 704:

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



Electron density around MTA A 705:

$2mF_o$-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.