



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2014 – 06:32 AM EDT

PDB ID : 4KTV
Title : Structural insights of MAT enzymes: MATa2b complexed with adenosine and pyrophosphate
Authors : Murray, B.; Antonyuk, S.V.; Marina, A.; Lu, S.C.; Mato, J.M.; Hasnain, S.S.; Rojas, A.L.
Deposited on : 2013-05-21
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

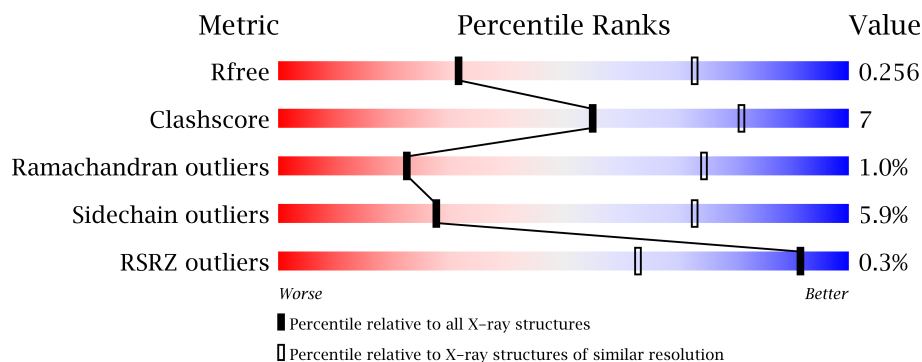
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	396	
1	B	396	
1	C	396	
1	D	396	
2	E	327	
2	F	327	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	A	402	-	X
3	EDO	B	401	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	B	403	-	X
3	EDO	C	401	-	X
3	EDO	D	401	-	X
3	EDO	D	402	-	X
3	EDO	D	403	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16508 atoms, of which 0 are hydrogen and 0 are deuterium.

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 S-adenosylmethionine synthase isoform type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2822	1790	492	529	11			
1	B	381	Total	C	N	O	S	0	0	0
			2963	1872	518	562	11			
1	C	361	Total	C	N	O	S	0	0	0
			2815	1785	491	528	11			
1	D	381	Total	C	N	O	S	0	0	0
			2963	1872	518	562	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P31153
B	0	SER	-	EXPRESSION TAG	UNP P31153
C	0	SER	-	EXPRESSION TAG	UNP P31153
D	0	SER	-	EXPRESSION TAG	UNP P31153

- Molecule 2 is a protein called Methionine adenosyltransferase 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	309	Total	C	N	O	S	0	0	0
			2448	1546	446	446	10			
2	F	295	Total	C	N	O	S	0	1	0
			2359	1493	431	425	10			

There are 8 discrepancies between the modelled and reference sequences:

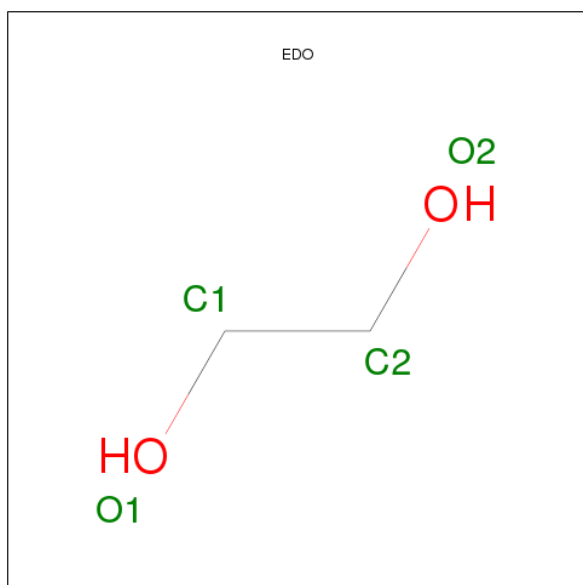
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP Q9NZL9
E	-2	SER	-	EXPRESSION TAG	UNP Q9NZL9
E	-1	HIS	-	EXPRESSION TAG	UNP Q9NZL9
E	0	MET	-	EXPRESSION TAG	UNP Q9NZL9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	EXPRESSION TAG	UNP Q9NZL9
F	-2	SER	-	EXPRESSION TAG	UNP Q9NZL9
F	-1	HIS	-	EXPRESSION TAG	UNP Q9NZL9
F	0	MET	-	EXPRESSION TAG	UNP Q9NZL9

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



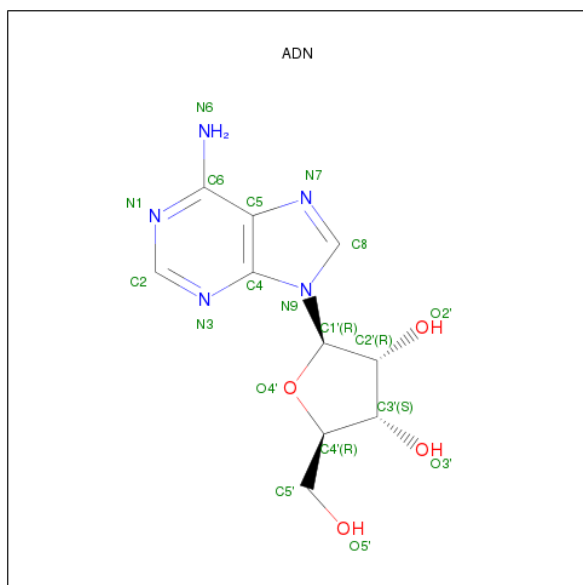
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

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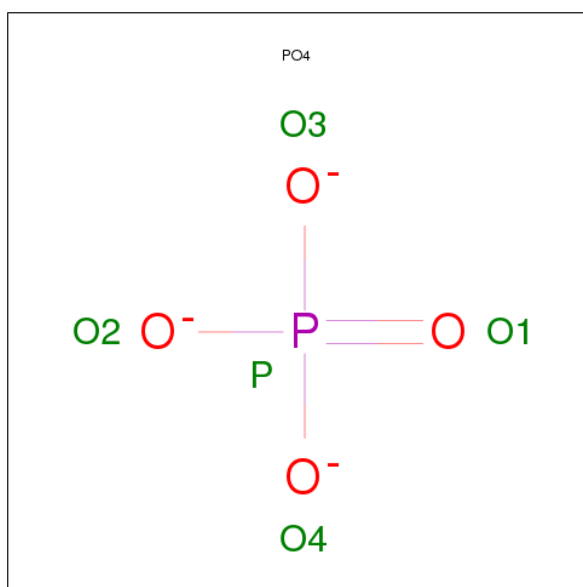
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$).



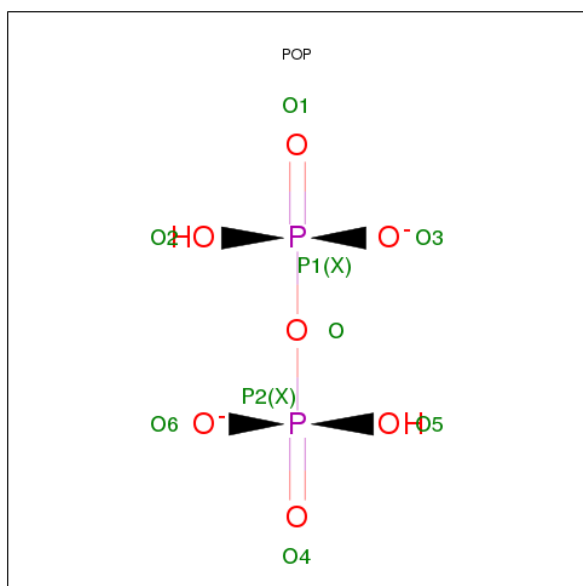
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	10	5	4		
4	C	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			9	7	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Mg 1 1	0	0

- Molecule 8 is water.

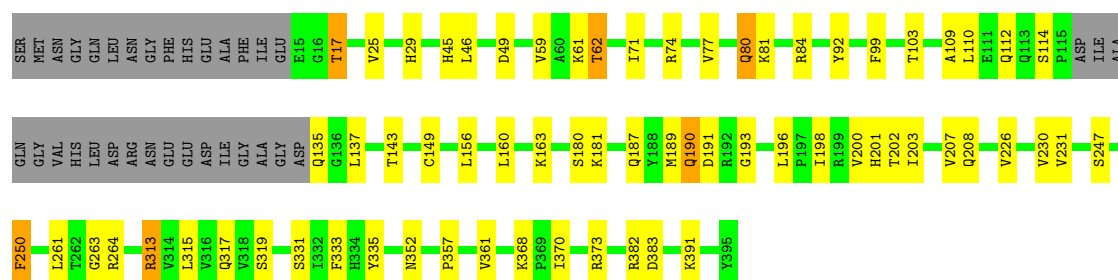
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	7	Total O 7 7	0	0
8	B	8	Total O 8 8	0	0
8	C	4	Total O 4 4	0	0
8	D	13	Total O 13 13	0	0
8	E	3	Total O 3 3	0	0
8	F	2	Total O 2 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

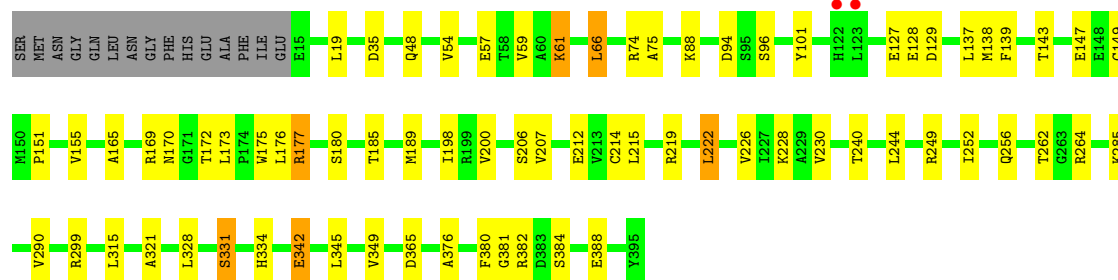
- Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain A:



- Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain B:



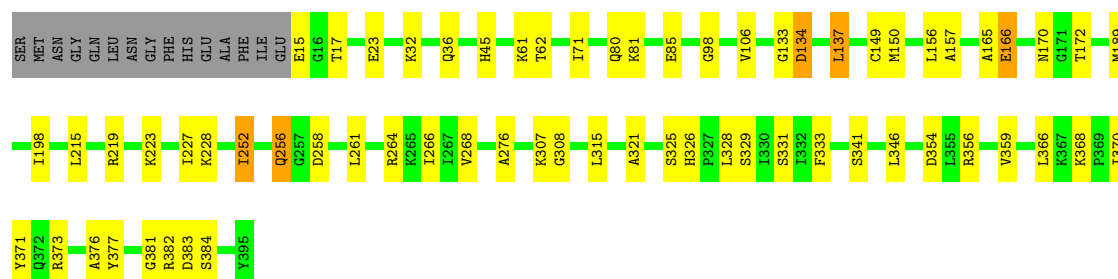
- Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain C:



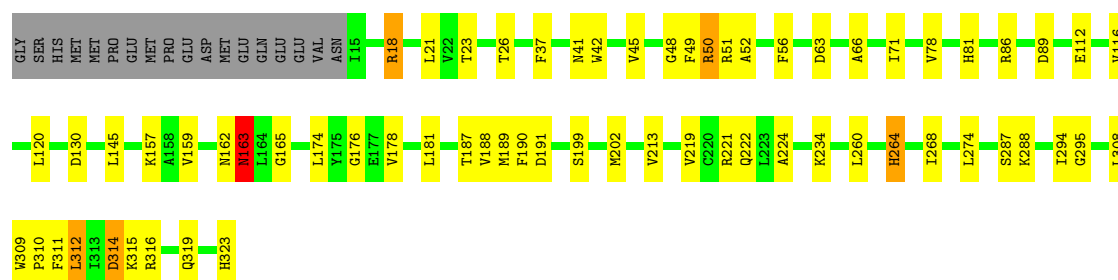
- Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain D:



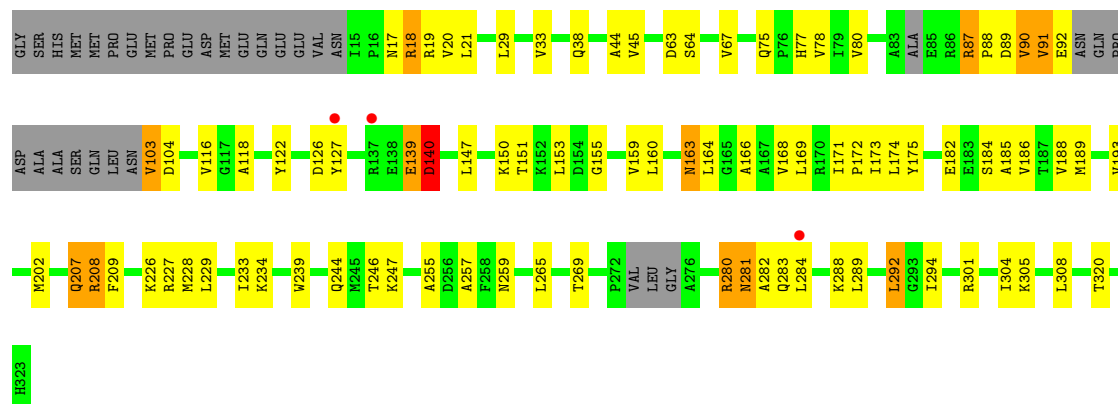
- Molecule 2: Methionine adenosyltransferase 2 subunit beta

Chain E:



- Molecule 2: Methionine adenosyltransferase 2 subunit beta

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.09Å 116.57Å 299.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.87 – 3.30 108.63 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (108.87-3.30) 99.8 (108.63-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.176 , 0.260 0.178 , 0.256	Depositor DCC
R_{free} test set	1949 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 38907 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16508	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, MG, PO4, POP, EDO

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	0.41	0/2879	0.63	0/3893
1	B	0.42	0/3022	0.64	0/4088
1	C	0.40	0/2871	0.63	0/3881
1	D	0.43	0/3022	0.64	0/4088
2	E	0.40	0/2507	0.62	0/3401
2	F	0.40	0/2417	0.63	0/3271
All	All	0.41	0/16718	0.63	0/22622

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2822	0	2832	41	0
1	B	2963	0	2956	38	0
1	C	2815	0	2825	28	0
1	D	2963	0	2956	35	0
2	E	2448	0	2418	34	0
2	F	2359	0	2335	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	12	0	0
3	B	16	0	24	1	0
3	C	8	0	12	0	0
3	D	12	0	18	2	0
3	E	4	0	6	0	0
4	A	19	0	13	2	0
4	C	19	0	13	0	0
5	A	5	0	0	0	0
6	C	9	0	0	0	0
7	D	1	0	0	0	0
8	A	7	0	0	0	0
8	B	8	0	0	0	0
8	C	4	0	0	0	0
8	D	13	0	0	0	0
8	E	3	0	0	0	0
8	F	2	0	0	0	0
All	All	16508	0	16420	220	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (220) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:MET:HB2	1:A:198:ILE:HD11	1.66	0.77
1:D:189:MET:HB2	1:D:198:ILE:HD11	1.67	0.77
1:A:25:VAL:HG12	1:A:181:LYS:HG2	1.64	0.77
1:C:200:VAL:HG23	1:C:235:TYR:HB3	1.72	0.72
1:C:48:GLN:HB2	1:C:75:ALA:HB2	1.72	0.71
2:F:168:VAL:HG12	2:F:168:VAL:O	1.92	0.70
1:A:156:LEU:HD22	1:A:231:VAL:HG22	1.77	0.65
1:A:45:HIS:CD2	1:A:77:VAL:HG21	2.32	0.65
2:F:126:ASP:HB3	2:F:284:LEU:HD21	1.79	0.65
1:D:321:ALA:HB2	1:D:328:LEU:HD11	1.78	0.64
2:E:78:VAL:HG21	2:E:224:ALA:HB1	1.79	0.64
1:C:45:HIS:CD2	1:C:77:VAL:HG21	2.32	0.64
2:F:88:PRO:HA	2:F:89:ASP:C	2.19	0.64
2:E:174:LEU:HD13	2:E:213:VAL:HG12	1.79	0.63
2:F:103:VAL:N	2:F:104:ASP:HA	2.14	0.63
2:F:226:LYS:O	2:F:226:LYS:HD3	1.99	0.62
1:A:59:VAL:HG21	1:B:59:VAL:HG21	1.83	0.61
1:A:373:ARG:O	1:A:382:ARG:NH2	2.34	0.60
1:A:109:ALA:HB1	1:B:61:LYS:HE2	1.83	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:19:ARG:NH1	2:F:75:GLN:O	2.35	0.59
1:B:200:VAL:O	1:B:240:THR:HG23	2.04	0.57
2:F:184:SER:O	2:F:188:VAL:HG13	2.03	0.57
1:A:370:ILE:HB	1:A:373:ARG:HE	1.69	0.57
1:B:376:ALA:O	1:B:382:ARG:NH2	2.37	0.57
1:A:261:LEU:HD11	1:B:57:GLU:HB3	1.87	0.57
1:C:261:LEU:HB3	1:D:261:LEU:HD13	1.87	0.57
1:B:334:HIS:CD2	1:B:342:GLU:HG3	2.39	0.57
1:C:267:ILE:HG22	1:C:272:GLY:HA2	1.87	0.57
1:A:352:ASN:O	1:A:391:LYS:HE3	2.05	0.56
1:A:137:LEU:HD11	1:A:317:GLN:CG	2.36	0.56
2:E:116:VAL:HG12	2:E:116:VAL:O	2.06	0.56
2:E:176:GLY:O	2:E:178:VAL:HG13	2.06	0.55
2:E:219:VAL:HG22	2:E:295:GLY:HA2	1.88	0.55
1:D:252:ILE:O	1:D:252:ILE:HG23	2.07	0.55
2:E:18:ARG:NH1	2:E:41:ASN:O	2.40	0.55
2:F:173:ILE:HD11	2:F:185:ALA:HB3	1.89	0.55
2:F:207:GLN:HA	2:F:246:THR:HG22	1.87	0.55
1:B:189:MET:HB2	1:B:198:ILE:HD11	1.88	0.54
2:F:63:ASP:O	2:F:67:VAL:HG23	2.07	0.54
1:A:137:LEU:HD11	1:A:317:GLN:HG2	1.89	0.54
1:D:98:GLY:O	1:D:256:GLN:HG2	2.07	0.54
1:B:48:GLN:HB2	1:B:75:ALA:HB2	1.88	0.54
1:A:59:VAL:HG22	1:A:261:LEU:HD22	1.89	0.54
1:B:345:LEU:O	1:B:349:VAL:HG23	2.08	0.54
2:F:257:ALA:HB1	2:F:305:LYS:HD2	1.90	0.53
1:D:346:LEU:HD22	3:D:403:EDO:H12	1.89	0.53
2:F:20:VAL:HA	2:F:78:VAL:O	2.08	0.53
2:F:116:VAL:HG12	2:F:116:VAL:O	2.09	0.53
2:F:87:ARG:O	2:F:89:ASP:HB3	2.09	0.52
2:F:292:LEU:N	2:F:292:LEU:HD22	2.24	0.52
2:E:37:PHE:CZ	2:E:221:ARG:HA	2.44	0.52
2:E:23:THR:OG1	2:E:81:HIS:HA	2.10	0.52
1:B:94:ASP:OD2	1:B:96:SER:HB2	2.10	0.52
2:F:182:GLU:HA	2:F:188:VAL:HG12	1.91	0.52
1:C:45:HIS:CE1	1:C:71:ILE:HG21	2.45	0.51
1:B:74:ARG:CZ	1:B:74:ARG:HB2	2.40	0.51
1:C:143:THR:O	1:C:149:CYS:HA	2.11	0.51
2:F:155:GLY:O	2:F:159:VAL:HG23	2.09	0.51
1:A:59:VAL:HG22	1:A:261:LEU:CD2	2.41	0.51
1:C:262:THR:O	1:D:264:ARG:NH1	2.44	0.51
1:B:151:PRO:O	1:B:155:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:346:LEU:HD22	3:D:403:EDO:C1	2.41	0.51
1:B:88:LYS:HG3	1:B:101:TYR:CE1	2.45	0.51
2:F:226:LYS:CD	2:F:226:LYS:O	2.60	0.50
1:A:200:VAL:HG11	1:A:203:ILE:HD11	1.93	0.50
1:C:311:CYS:HB3	1:C:338:SER:HB2	1.93	0.50
1:A:143:THR:O	1:A:149:CYS:HA	2.12	0.50
2:F:122:TYR:CD1	2:F:159:VAL:HG21	2.46	0.50
1:C:226:VAL:O	1:C:230:VAL:HG23	2.11	0.50
1:D:45:HIS:CE1	1:D:71:ILE:HG21	2.46	0.50
2:E:71:ILE:HG22	2:E:116:VAL:HG21	1.94	0.50
1:A:160:LEU:HD23	1:A:230:VAL:HG21	1.94	0.50
2:F:163:ASN:ND2	2:F:166:ALA:HB2	2.27	0.50
1:B:331:SER:HA	3:B:401:EDO:C2	2.42	0.49
2:F:21:LEU:HD12	2:F:45:VAL:O	2.12	0.49
1:C:144:ASP:OD2	1:C:312:ARG:HB3	2.12	0.49
2:E:52:ALA:HB1	2:E:56:PHE:HB2	1.93	0.49
2:E:120:LEU:HD23	2:E:159:VAL:HG13	1.94	0.49
2:F:103:VAL:N	2:F:104:ASP:CA	2.75	0.49
2:F:160:LEU:HD11	2:F:168:VAL:HG21	1.95	0.49
2:E:315:LYS:O	2:E:319:GLN:HG3	2.11	0.49
2:F:168:VAL:CG1	2:F:168:VAL:O	2.60	0.49
2:F:169:LEU:HD11	2:F:239:TRP:HB3	1.95	0.48
2:F:281:ASN:OD1	2:F:282:ALA:N	2.46	0.48
1:B:226:VAL:O	1:B:230:VAL:HG23	2.12	0.48
2:F:288:LYS:O	2:F:292:LEU:HD21	2.13	0.48
1:D:23:GLU:O	1:D:268:VAL:HG22	2.13	0.48
2:E:309:TRP:HA	2:E:312:LEU:HD22	1.94	0.48
1:C:202:THR:HG21	1:D:328:LEU:HD13	1.94	0.48
1:C:334:HIS:O	1:C:337:THR:OG1	2.29	0.48
1:D:307:LYS:O	1:D:308:GLY:C	2.51	0.48
2:F:292:LEU:H	2:F:292:LEU:HD22	1.77	0.48
1:C:265:LYS:HB3	1:C:268:VAL:HB	1.95	0.48
1:B:165:ALA:HB1	1:B:169:ARG:HH21	1.79	0.48
1:D:80:GLN:HE22	1:D:106:VAL:HB	1.78	0.47
2:F:173:ILE:HD12	2:F:208:ARG:NH1	2.29	0.47
1:C:354:ASP:HB3	1:C:359:VAL:HG11	1.95	0.47
1:A:109:ALA:HB1	1:B:61:LYS:CE	2.45	0.47
1:D:354:ASP:HB3	1:D:359:VAL:HG11	1.97	0.47
1:D:366:LEU:O	1:D:371:TYR:OH	2.28	0.47
1:A:193:GLY:O	1:A:313:ARG:NH1	2.48	0.47
1:A:370:ILE:HB	1:A:373:ARG:NE	2.28	0.47
1:B:48:GLN:HB2	1:B:75:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:326:HIS:CD2	1:D:356:ARG:HD3	2.50	0.46
1:C:353:PHE:HB3	1:C:355:LEU:HD21	1.96	0.46
2:F:227:ARG:HD3	2:F:233:ILE:HB	1.95	0.46
1:A:180:SER:HB3	1:A:207:VAL:HG23	1.98	0.46
1:D:170:ASN:C	1:D:170:ASN:OD1	2.54	0.46
2:E:130:ASP:HB2	2:E:145:LEU:HD21	1.98	0.46
2:F:33:VAL:HG11	2:F:80:VAL:HG11	1.97	0.46
2:E:18:ARG:HB2	2:E:42:TRP:CE3	2.51	0.46
2:F:139:GLU:O	2:F:140:ASP:O	2.33	0.46
2:F:89:ASP:O	2:F:91:VAL:HG23	2.16	0.46
1:B:299:ARG:HG2	1:B:380:PHE:CD1	2.51	0.46
1:B:54:VAL:O	1:B:285:LYS:HA	2.16	0.46
1:D:215:LEU:HD23	1:D:219:ARG:NH2	2.31	0.46
2:E:49:PHE:O	2:E:50:ARG:C	2.54	0.46
1:B:180:SER:HB3	1:B:207:VAL:HG23	1.98	0.46
1:B:321:ALA:HB2	1:B:328:LEU:HD21	1.98	0.45
1:D:137:LEU:N	1:D:137:LEU:HD23	2.30	0.45
2:F:280:ARG:O	2:F:281:ASN:CB	2.64	0.45
2:E:21:LEU:HD12	2:E:45:VAL:O	2.16	0.45
2:F:18:ARG:HB2	2:F:18:ARG:CZ	2.46	0.45
1:B:215:LEU:HG	1:B:219:ARG:HE	1.81	0.45
1:D:370:ILE:HB	1:D:373:ARG:HD2	1.98	0.45
1:B:165:ALA:HB1	1:B:169:ARG:NH2	2.31	0.45
1:B:381:GLY:H	1:B:388:GLU:CD	2.19	0.45
1:A:247:SER:CB	4:A:403:ADN:N1	2.80	0.45
1:A:74:ARG:CZ	1:A:74:ARG:HB2	2.47	0.45
2:F:202:MET:CE	2:F:265:LEU:HD22	2.47	0.45
2:F:226:LYS:HE2	2:F:292:LEU:HG	1.98	0.45
2:F:88:PRO:HA	2:F:90:VAL:N	2.32	0.45
1:C:175:TRP:HB2	1:C:210:ASP:OD1	2.17	0.45
1:C:48:GLN:HB2	1:C:75:ALA:CB	2.44	0.45
2:E:181:LEU:HD21	2:E:311:PHE:CG	2.52	0.44
1:A:163:LYS:HG2	1:A:226:VAL:HG13	1.99	0.44
2:E:188:VAL:C	2:E:190:PHE:H	2.20	0.44
1:B:143:THR:O	1:B:149:CYS:HA	2.17	0.44
1:C:271:TYR:O	1:C:274:TRP:N	2.48	0.44
1:D:165:ALA:O	1:D:166:GLU:C	2.56	0.44
2:E:48:GLY:O	2:E:52:ALA:HB2	2.17	0.44
2:F:189:MET:O	2:F:193:VAL:HG23	2.18	0.44
1:D:133:GLY:O	1:D:134:ASP:HB2	2.17	0.44
1:D:223:LYS:HA	1:D:227:ILE:HD12	1.99	0.44
2:E:188:VAL:O	2:E:190:PHE:N	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:176:LEU:C	1:B:177:ARG:HG2	2.38	0.44
1:B:35:ASP:HA	1:B:262:THR:HG23	1.98	0.44
1:C:299:ARG:HG2	1:C:380:PHE:CD1	2.53	0.44
1:A:71:ILE:O	1:A:112:GLN:HA	2.18	0.44
1:C:165:ALA:HB1	1:C:169:ARG:NH2	2.33	0.44
2:E:222:GLN:HB3	2:E:294:ILE:HG23	2.00	0.44
2:F:294:ILE:HG22	2:F:294:ILE:O	2.18	0.44
1:B:138:MET:N	1:B:138:MET:SD	2.91	0.44
1:D:150:MET:HG3	1:D:381:GLY:HA3	2.00	0.44
1:A:61:LYS:O	1:A:62:THR:C	2.56	0.44
2:F:92:GLU:HB3	2:F:147:LEU:HD12	2.00	0.44
2:E:199:SER:HA	2:E:264:HIS:HB2	2.00	0.43
2:F:104:ASP:C	2:F:104:ASP:OD2	2.57	0.43
1:A:201:HIS:ND1	1:A:202:THR:OG1	2.44	0.43
2:F:38:GLN:HB2	2:F:44:ALA:HB3	2.01	0.43
2:E:287:SER:O	2:E:288:LYS:C	2.57	0.43
2:E:314:ASP:OD2	2:E:314:ASP:N	2.46	0.43
2:F:304:ILE:HG13	2:F:308:LEU:HD12	1.99	0.43
2:F:175:TYR:HB3	2:F:186:VAL:HG21	2.00	0.43
1:A:190:GLN:HE21	1:A:191:ASP:N	2.17	0.43
1:C:391:LYS:O	1:C:393:LEU:HD22	2.18	0.43
1:D:376:ALA:O	1:D:377:TYR:HB2	2.18	0.43
1:A:46:LEU:HA	1:A:49:ASP:O	2.18	0.43
1:C:165:ALA:HB1	1:C:169:ARG:HH21	1.84	0.43
1:C:352:ASN:HD21	1:C:394:LYS:H	1.66	0.43
1:D:81:LYS:O	1:D:85:GLU:HG2	2.18	0.43
1:A:208:GLN:HA	1:A:250:PHE:O	2.19	0.42
1:C:15:GLU:N	1:C:15:GLU:CD	2.72	0.42
2:F:87:ARG:HD3	2:F:184:SER:HA	2.00	0.42
1:D:383:ASP:O	1:D:384:SER:HB2	2.19	0.42
2:E:165:GLY:HA2	2:E:234:LYS:HB2	2.00	0.42
2:E:309:TRP:N	2:E:310:PRO:CD	2.82	0.42
1:A:25:VAL:HG12	1:A:181:LYS:CG	2.43	0.42
1:B:222:LEU:O	1:B:226:VAL:HB	2.20	0.42
1:B:170:ASN:OD1	1:B:172:THR:HG22	2.19	0.42
1:B:66:LEU:O	1:B:66:LEU:HD23	2.19	0.42
1:D:150:MET:HE2	1:D:150:MET:HA	2.02	0.42
1:D:156:LEU:O	1:D:157:ALA:C	2.58	0.42
1:D:276:ALA:HB2	2:E:323:HIS:CE1	2.54	0.42
1:A:357:PRO:O	1:A:361:VAL:HG13	2.20	0.42
1:A:261:LEU:HD12	1:A:264:ARG:HH11	1.85	0.42
2:F:29:LEU:O	2:F:33:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:92:TYR:HB3	1:A:99:PHE:HB3	2.03	0.41
1:B:66:LEU:C	1:B:66:LEU:HD23	2.41	0.41
1:C:27:GLU:OE2	1:C:169:ARG:NH2	2.44	0.41
1:D:150:MET:CE	1:D:150:MET:HA	2.50	0.41
2:E:162:ASN:O	2:E:163:ASN:HB2	2.20	0.41
2:F:289:LEU:HD11	2:F:294:ILE:HG21	2.03	0.41
2:E:130:ASP:CB	2:E:145:LEU:HD21	2.50	0.41
2:E:191:ASP:OD1	2:E:316:ARG:NH2	2.41	0.41
2:F:126:ASP:CB	2:F:284:LEU:HD21	2.49	0.41
1:A:80:GLN:HG3	1:A:84:ARG:HE	1.85	0.41
1:B:19:LEU:HD22	1:B:185:THR:HG22	2.02	0.41
1:C:88:LYS:HG3	1:C:101:TYR:CE1	2.55	0.41
2:E:163:ASN:HD22	2:E:163:ASN:C	2.23	0.41
1:A:17:THR:HG21	1:A:187:GLN:HE21	1.86	0.41
1:A:29:HIS:CD2	4:A:403:ADN:O2'	2.73	0.41
1:B:94:ASP:OD2	1:B:96:SER:CB	2.69	0.41
1:A:103:THR:O	1:D:62:THR:HG22	2.21	0.41
2:F:171:ILE:CD1	2:F:174:LEU:HD11	2.50	0.41
2:E:63:ASP:OD2	2:E:66:ALA:HB2	2.21	0.41
1:B:173:LEU:HD22	1:B:175:TRP:CZ2	2.56	0.41
1:A:263:GLY:O	1:B:264:ARG:HD3	2.20	0.41
2:F:207:GLN:HG2	2:F:244:GLN:HE21	1.86	0.41
1:B:139:PHE:CD1	1:B:315:LEU:HD11	2.56	0.41
1:C:266:ILE:HD11	1:D:266:ILE:HD11	2.03	0.41
1:D:315:LEU:HB3	1:D:333:PHE:HB2	2.02	0.41
1:D:36:GLN:HE21	1:D:36:GLN:HB2	1.71	0.41
2:F:77:HIS:O	2:F:118:ALA:HA	2.21	0.40
2:F:89:ASP:O	2:F:90:VAL:C	2.59	0.40
2:F:288:LYS:O	2:F:292:LEU:CD2	2.68	0.40
1:A:315:LEU:HD23	1:A:333:PHE:HD2	1.86	0.40
1:A:71:ILE:HD12	1:A:110:LEU:HD13	2.03	0.40
2:F:255:ALA:O	2:F:259:ASN:N	2.55	0.40
2:E:187:THR:HG22	2:E:308:LEU:HD21	2.04	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	358/396 (90%)	330 (92%)	26 (7%)	2 (1%)	33	83
1	B	379/396 (96%)	349 (92%)	29 (8%)	1 (0%)	50	92
1	C	357/396 (90%)	322 (90%)	33 (9%)	2 (1%)	33	83
1	D	379/396 (96%)	343 (90%)	33 (9%)	3 (1%)	27	78
2	E	307/327 (94%)	281 (92%)	22 (7%)	4 (1%)	18	69
2	F	288/327 (88%)	238 (83%)	42 (15%)	8 (3%)	8	48
All	All	2068/2238 (92%)	1863 (90%)	185 (9%)	20 (1%)	22	74

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	272	GLY
2	E	50	ARG
2	E	163	ASN
2	F	140	ASP
1	A	335	TYR
1	C	62	THR
1	D	134	ASP
2	F	281	ASN
1	A	62	THR
1	D	172	THR
2	E	189	MET
2	F	234	LYS
2	F	283	GLN
2	F	127	TYR
1	D	252	ILE
2	E	264	HIS
2	F	90	VAL
2	F	172	PRO
1	B	252	ILE
2	F	91	VAL

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	302/328 (92%)	289 (96%)	13 (4%)	40	82
1	B	316/328 (96%)	295 (93%)	21 (7%)	24	68
1	C	301/328 (92%)	284 (94%)	17 (6%)	30	75
1	D	316/328 (96%)	300 (95%)	16 (5%)	33	77
2	E	262/279 (94%)	248 (95%)	14 (5%)	32	76
2	F	253/279 (91%)	230 (91%)	23 (9%)	14	49
All	All	1750/1870 (94%)	1646 (94%)	104 (6%)	28	73

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

Mol	Chain	Res	Type
1	A	17	THR
1	A	80	GLN
1	A	81	LYS
1	A	114	SER
1	A	135	GLN
1	A	190	GLN
1	A	196	LEU
1	A	250	PHE
1	A	313	ARG
1	A	319	SER
1	A	331	SER
1	A	368	LYS
1	A	383	ASP
1	B	61	LYS
1	B	66	LEU
1	B	127	GLU
1	B	128	GLU
1	B	129	ASP
1	B	137	LEU
1	B	147	GLU
1	B	177	ARG
1	B	206	SER
1	B	212	GLU
1	B	214	CYS
1	B	222	LEU
1	B	228	LYS
1	B	244	LEU

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Mol	Chain	Res	Type
1	B	249	ARG
1	B	256	GLN
1	B	290	VAL
1	B	331	SER
1	B	342	GLU
1	B	365	ASP
1	B	384	SER
1	C	15	GLU
1	C	61	LYS
1	C	81	LYS
1	C	113	GLN
1	C	138	MET
1	C	148	GLU
1	C	149	CYS
1	C	191	ASP
1	C	206	SER
1	C	228	LYS
1	C	250	PHE
1	C	326	HIS
1	C	328	LEU
1	C	339	GLN
1	C	347	GLU
1	C	382	ARG
1	C	384	SER
1	D	15	GLU
1	D	17	THR
1	D	32	LYS
1	D	61	LYS
1	D	137	LEU
1	D	149	CYS
1	D	166	GLU
1	D	228	LYS
1	D	256	GLN
1	D	258	ASP
1	D	325	SER
1	D	329	SER
1	D	331	SER
1	D	341	SER
1	D	368	LYS
1	D	382	ARG
2	E	18	ARG
2	E	26	THR

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Mol	Chain	Res	Type
2	E	51	ARG
2	E	86	ARG
2	E	89	ASP
2	E	112	GLU
2	E	157	LYS
2	E	163	ASN
2	E	202	MET
2	E	260	LEU
2	E	268	ILE
2	E	274	LEU
2	E	312	LEU
2	E	314	ASP
2	F	17	ASN
2	F	18	ARG
2	F	64	SER
2	F	87	ARG
2	F	103	VAL
2	F	139	GLU
2	F	140	ASP
2	F	150	LYS
2	F	151	THR
2	F	153	LEU
2	F	163	ASN
2	F	164	LEU
2	F	207	GLN
2	F	208	ARG
2	F	209	PHE
2	F	228	MET
2	F	229	LEU
2	F	247	LYS
2	F	269	THR
2	F	280	ARG
2	F	292	LEU
2	F	301	ARG
2	F	320	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	161	ASN
1	A	170	ASN

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Mol	Chain	Res	Type
1	A	190	GLN
1	B	113	GLN
1	B	190	GLN
1	B	317	GLN
1	C	45	HIS
1	C	48	GLN
1	C	89	HIS
1	C	113	GLN
1	C	339	GLN
1	C	352	ASN
1	D	36	GLN
1	D	113	GLN
1	D	256	GLN
2	E	41	ASN
2	E	65	ASN
2	E	100	GLN
2	E	163	ASN
2	F	40	ASN
2	F	108	ASN
2	F	163	ASN
2	F	244	GLN
2	F	264	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	401	-	3,3,3	0.54	0	2,2,2	0.27	0
3	EDO	A	402	-	3,3,3	0.60	0	2,2,2	0.16	0
4	ADN	A	403	-	21,21,21	1.26	3 (14%)	31,31,31	2.32	8 (25%)
5	PO4	A	404	-	4,4,4	0.23	0	6,6,6	0.29	0
3	EDO	B	401	-	3,3,3	0.50	0	2,2,2	0.58	0
3	EDO	B	402	-	3,3,3	0.49	0	2,2,2	0.37	0
3	EDO	B	403	-	3,3,3	0.45	0	2,2,2	0.47	0
3	EDO	B	404	-	3,3,3	0.54	0	2,2,2	0.29	0
3	EDO	C	401	-	3,3,3	0.42	0	2,2,2	0.44	0
3	EDO	C	402	-	3,3,3	0.61	0	2,2,2	0.28	0
4	ADN	C	403	-	21,21,21	1.30	3 (14%)	31,31,31	2.29	6 (19%)
6	POP	C	404	7	8,8,8	0.66	0	13,13,13	0.94	0
3	EDO	D	401	-	3,3,3	0.53	0	2,2,2	0.41	0
3	EDO	D	402	-	3,3,3	0.63	0	2,2,2	0.22	0
3	EDO	D	403	-	3,3,3	0.45	0	2,2,2	0.58	0
3	EDO	E	401	-	3,3,3	0.49	0	2,2,2	0.41	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	EDO	A	401	-	-	0/1/1/1	0/0/0/0
3	EDO	A	402	-	-	0/1/1/1	0/0/0/0
4	ADN	A	403	-	-	0/6/22/22	0/3/3/3
5	PO4	A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	B	401	-	-	0/1/1/1	0/0/0/0
3	EDO	B	402	-	-	0/1/1/1	0/0/0/0
3	EDO	B	403	-	-	0/1/1/1	0/0/0/0
3	EDO	B	404	-	-	0/1/1/1	0/0/0/0
3	EDO	C	401	-	-	0/1/1/1	0/0/0/0
3	EDO	C	402	-	-	0/1/1/1	0/0/0/0
4	ADN	C	403	-	-	0/6/22/22	0/3/3/3
6	POP	C	404	7	-	0/6/6/6	0/0/0/0
3	EDO	D	401	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	402	-	-	0/1/1/1	0/0/0/0
3	EDO	D	403	-	-	0/1/1/1	0/0/0/0
3	EDO	E	401	-	-	0/1/1/1	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	ADN	C5-C4	3.31	1.48	1.40
4	C	403	ADN	C5-C4	3.19	1.47	1.40
4	A	403	ADN	C4-N9	-3.04	1.33	1.37
4	C	403	ADN	C4-N9	-2.93	1.33	1.37
4	C	403	ADN	O4'-C1'	2.41	1.44	1.41
4	A	403	ADN	O4'-C1'	2.24	1.44	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	ADN	N3-C2-N1	-7.48	122.31	128.89
4	C	403	ADN	C5-C4-N3	-7.15	119.01	125.98
4	C	403	ADN	N3-C2-N1	-6.20	123.44	128.89
4	A	403	ADN	C5-C4-N3	-5.71	120.41	125.98
4	C	403	ADN	N3-C4-N9	5.49	134.81	125.39
4	A	403	ADN	N3-C4-N9	4.87	133.74	125.39
4	A	403	ADN	C2-N1-C6	2.80	123.74	118.76
4	A	403	ADN	C1'-N9-C4	-2.50	122.32	126.64
4	A	403	ADN	C3'-C2'-C1'	2.49	104.82	100.92
4	C	403	ADN	C2-N3-C4	2.48	120.40	113.27
4	A	403	ADN	C2-N3-C4	2.42	120.23	113.27
4	C	403	ADN	C3'-C2'-C1'	2.31	104.55	100.92
4	A	403	ADN	C8-N9-C4	2.22	108.76	106.96
4	C	403	ADN	C4'-O4'-C1'	2.12	112.05	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	362/396 (91%)	-0.06	0 100 100	41, 59, 85, 110	0
1	B	381/396 (96%)	-0.01	2 (0%) 88 51	45, 61, 103, 159	0
1	C	361/396 (91%)	0.02	1 (0%) 91 63	42, 67, 96, 133	0
1	D	381/396 (96%)	-0.07	0 100 100	41, 55, 83, 116	0
2	E	309/327 (94%)	0.03	0 100 100	45, 67, 93, 118	0
2	F	295/327 (90%)	0.32	3 (1%) 79 33	47, 100, 132, 151	0
All	All	2089/2238 (93%)	0.03	6 (0%) 91 63	41, 65, 111, 159	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	HIS	3.9
1	B	123	LEU	3.7
1	C	323	GLY	2.5
2	F	284	LEU	2.1
2	F	137	ARG	2.1
2	F	127	TYR	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	A	402	4/4	0.39	8.73	71,74,75,76	0
3	EDO	D	401	4/4	0.56	6.80	68,68,68,68	0
3	EDO	B	403	4/4	0.36	4.56	81,81,82,85	0
3	EDO	D	402	4/4	0.36	4.27	67,68,68,71	0
3	EDO	D	403	4/4	0.41	2.85	62,64,64,64	0
3	EDO	C	401	4/4	0.39	2.65	65,67,68,74	0
3	EDO	B	401	4/4	0.28	2.39	54,57,60,64	0
4	ADN	A	403	19/19	0.47	1.67	97,127,138,138	0
3	EDO	B	404	4/4	0.47	1.32	85,87,90,93	0
3	EDO	B	402	4/4	0.26	0.99	58,58,58,59	0
6	POP	C	404	9/9	0.29	0.91	111,113,140,146	0
3	EDO	A	401	4/4	0.34	0.84	69,69,71,71	0
4	ADN	C	403	19/19	0.29	0.42	51,67,71,71	0
5	PO4	A	404	5/5	0.24	-0.16	119,125,132,133	0
7	MG	D	404	1/1	0.23	-0.29	49,49,49,49	0
3	EDO	E	401	4/4	0.15	-1.34	43,47,49,53	0
3	EDO	C	402	4/4	0.44	-	90,98,98,99	0

6.5 Other polymers ⓘ

There are no such residues in this entry.