



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:30 PM UTC

PDB ID : 1V2E / pdb_00001v2e
Title : Crystal Structure of T.th HB8 Glutamine Aminotransferase complex with a-k
eto-g-methylthiobutyrate
Authors : Goto, M.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2003-10-15
Resolution : 2.60 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

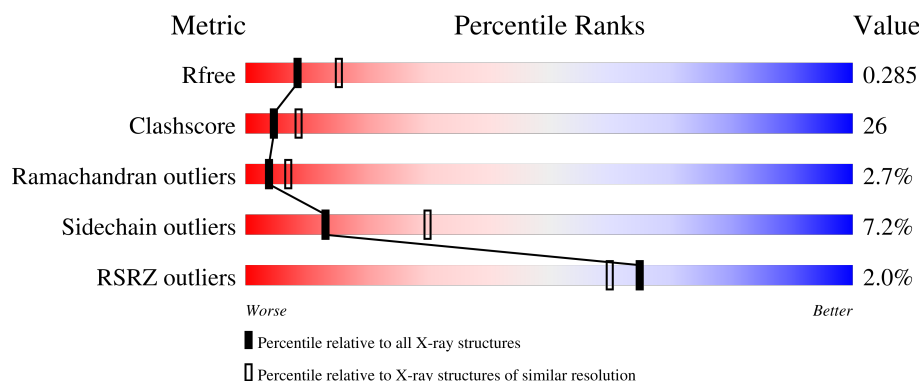
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	381	2% 56% 34% 6%
1	B	381	2% 45% 45% 6%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	KMT	A	520	-	X	-	-
3	KMT	B	1520	-	X	-	-

2 Entry composition [i](#)

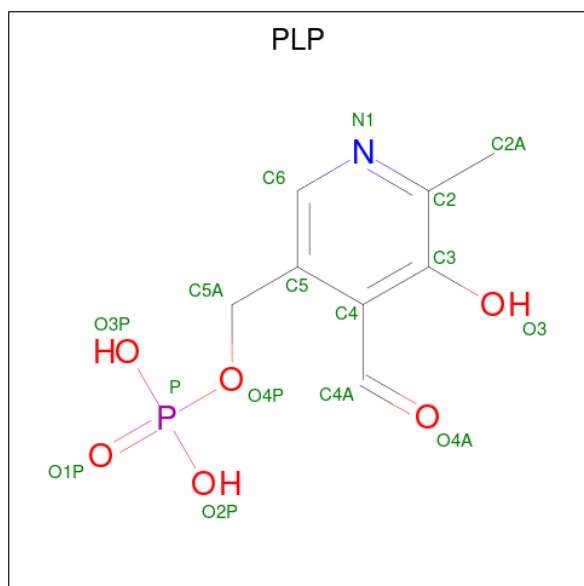
There are 4 unique types of molecules in this entry. The entry contains 5930 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamine Aminotransferase.

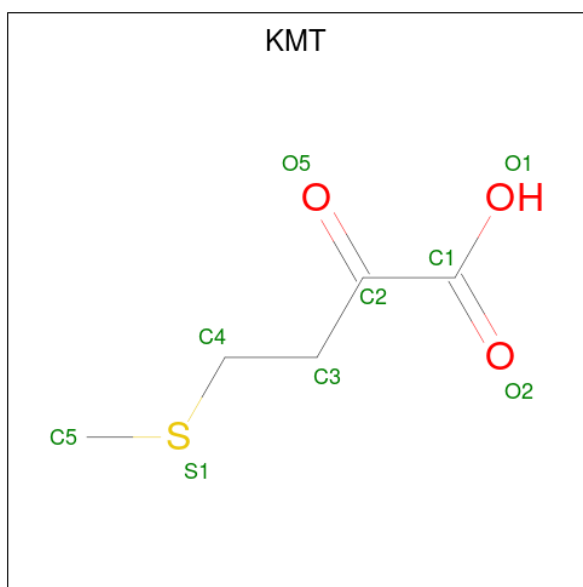
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2901	1864	513	516	8			
1	B	367	Total	C	N	O	S	0	0	0
			2894	1859	512	515	8			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 4-(METHYLSULFANYL)-2-OXOBUTANOIC ACID (CCD ID: KMT) (formula: $C_5H_8O_3S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			9	5	3	1		
3	B	1	Total	C	O	S	0	0
			9	5	3	1		

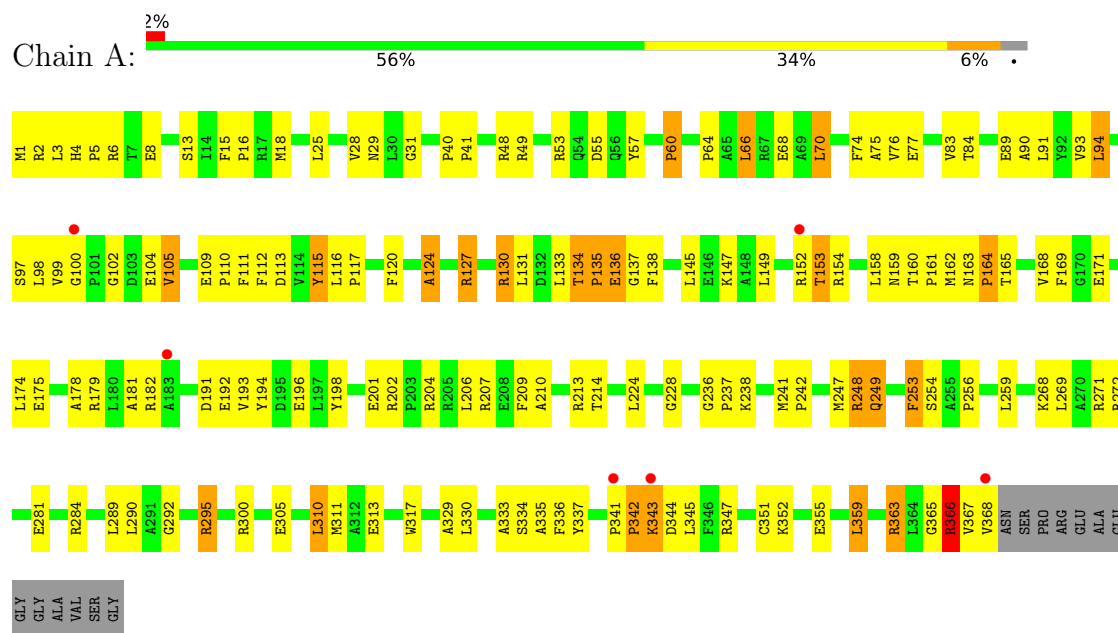
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	43	Total	O	0	0
			43	43		

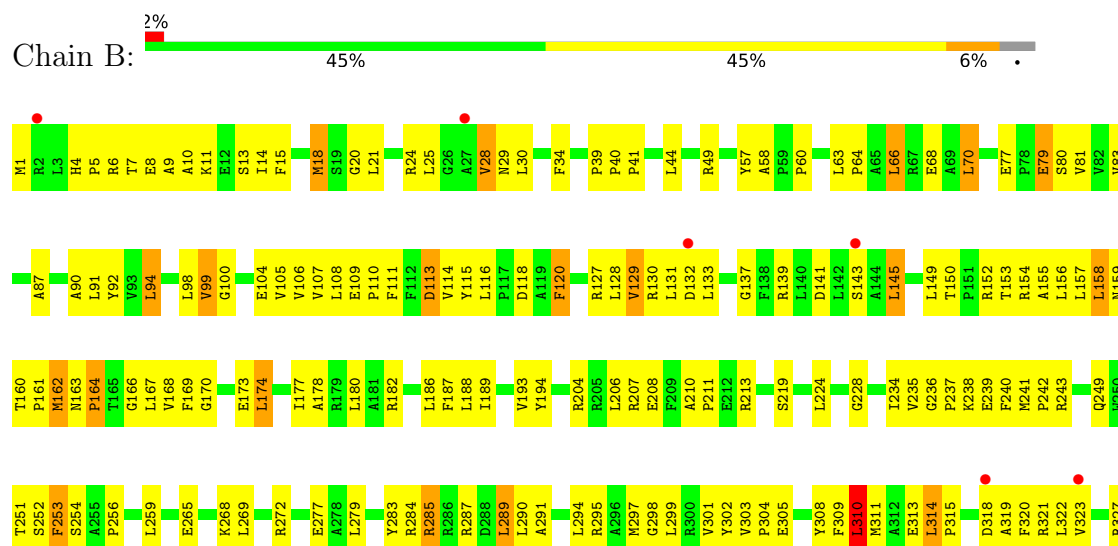
3 Residue-property plots [i](#)

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: Glutamine Aminotransferase



• Molecule 1: Glutamine Aminotransferase



Y328	F336	F339	F340	F341	F342	F343	F344	F345	F346	F347	F348	F349	F350	F351	F352	F353	F354	F355	F356	F357	F358	F359	F360	F361	F362	F363	F364	F365	F366	F367	VAL	ASN	SER	PRO	ARG	GLU	ALA	GLY	GLY	ALA	VAL	SER	GLY			

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.14Å 123.14Å 122.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60 10.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.60) 96.2 (10.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.231 , 0.286 0.229 , 0.285	Depositor DCC
R_{free} test set	3279 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5930	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KMT, PLP

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	0.50	0/2971	0.96	8/4031 (0.2%)
1	B	0.46	0/2964	0.97	11/4021 (0.3%)
All	All	0.48	0/5935	0.97	19/8052 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ALA	N-CA-C	-7.88	100.85	110.31
1	B	224	LEU	N-CA-C	7.36	121.56	112.59
1	B	115	TYR	N-CA-C	6.67	119.15	111.02
1	A	351	CYS	N-CA-C	-6.18	104.32	112.72
1	A	162	MET	N-CA-C	5.93	119.31	109.46
1	B	163	ASN	N-CA-C	-5.67	100.80	109.64
1	A	165	THR	N-CA-C	5.45	117.30	111.36
1	A	163	ASN	N-CA-C	-5.42	101.19	109.64
1	A	214	THR	N-CA-C	5.41	118.06	109.24
1	B	174	LEU	N-CA-C	-5.41	105.07	110.97
1	A	130	ARG	N-CA-C	5.39	117.52	109.59
1	A	224	LEU	N-CA-C	5.34	119.30	112.26
1	B	314	LEU	CA-C-N	5.31	126.48	119.84
1	B	314	LEU	C-N-CA	5.31	126.48	119.84
1	B	162	MET	N-CA-C	5.22	117.88	110.10
1	A	31	GLY	N-CA-C	5.14	114.88	110.21
1	B	303	VAL	CA-C-N	5.09	125.07	120.03
1	B	303	VAL	C-N-CA	5.09	125.07	120.03
1	B	99	VAL	N-CA-C	5.00	115.85	108.45

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	2901	0	2929	134	0
1	B	2894	0	2920	188	0
2	A	15	0	7	0	0
2	B	15	0	7	2	0
3	A	9	0	7	1	0
3	B	9	0	7	1	0
4	A	44	0	0	3	0
4	B	43	0	0	5	1
All	All	5930	0	5877	304	1

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 26.

All (304) 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:B:158:LEU:HD21	1:B:169:PHE:HE1	1.29	0.98
1:B:158:LEU:HD13	1:B:159:ASN:H	1.33	0.93
1:A:268:LYS:HE2	1:A:268:LYS:HA	1.53	0.90
1:A:174:LEU:HD12	1:A:206:LEU:HD13	1.56	0.87
1:B:39:PRO:HG2	1:B:44:LEU:HD21	1.60	0.82
1:B:114:VAL:HG12	1:B:118:ASP:OD2	1.77	0.81
1:A:249:GLN:HE22	1:B:13:SER:H	1.26	0.80
1:A:66:LEU:HD13	1:A:83:VAL:HG21	1.64	0.80
1:B:314:LEU:HG	4:B:1559:HOH:O	1.81	0.79
1:B:158:LEU:HD21	1:B:169:PHE:CE1	2.16	0.79
1:B:5:PRO:O	1:B:8:GLU:HG3	1.82	0.78
1:B:178:ALA:O	1:B:182:ARG:HG3	1.83	0.78
1:A:18:MET:HE2	1:A:330:LEU:O	1.83	0.78
1:A:168:VAL:HG23	1:A:305:GLU:HB2	1.67	0.77
1:A:66:LEU:HD22	1:A:70:LEU:HD22	1.65	0.77
1:B:158:LEU:HD13	1:B:159:ASN:N	2.01	0.75
1:B:313:GLU:HA	1:B:344:ASP:O	1.87	0.73
1:A:49:ARG:O	1:A:53:ARG:HD3	1.88	0.73
1:B:188:LEU:HD13	1:B:206:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD12	1:B:206:LEU:HD13	1.71	0.72
1:A:337:TYR:CE2	1:A:342:PRO:HD2	2.25	0.71
1:B:8:GLU:O	1:B:11:LYS:HE3	1.90	0.71
1:B:109:GLU:HB3	1:B:130:ARG:HA	1.71	0.71
1:A:178:ALA:HB1	1:A:210:ALA:HB2	1.73	0.70
1:A:158:LEU:HD12	1:A:206:LEU:HD22	1.71	0.70
1:B:168:VAL:HG23	1:B:305:GLU:HB2	1.74	0.70
1:A:99:VAL:HG11	1:A:105:VAL:HG22	1.74	0.70
1:B:295:ARG:HE	1:B:301:VAL:HB	1.59	0.68
1:A:158:LEU:HD22	1:A:169:PHE:HE1	1.60	0.66
1:A:249:GLN:HE22	1:B:13:SER:N	1.93	0.66
1:B:158:LEU:HD11	1:B:169:PHE:CD1	2.31	0.66
1:B:290:LEU:O	1:B:294:LEU:HG	1.96	0.66
1:A:292:GLY:HA2	1:A:295:ARG:NH1	2.10	0.66
1:A:363:ARG:HD3	4:A:529:HOH:O	1.94	0.66
1:A:109:GLU:O	1:A:131:LEU:HD13	1.96	0.66
1:B:108:LEU:HD13	1:B:131:LEU:HD11	1.78	0.65
1:A:295:ARG:HH11	1:A:295:ARG:HB2	1.59	0.65
1:B:299:LEU:HD13	1:B:313:GLU:O	1.97	0.65
1:B:186:LEU:O	1:B:213:ARG:HD3	1.97	0.65
1:B:80:SER:HB2	1:B:236:GLY:O	1.97	0.65
1:A:159:ASN:HD22	1:A:191:ASP:HB3	1.62	0.64
1:B:359:LEU:O	1:B:359:LEU:HD22	1.98	0.64
1:B:156:LEU:HD23	1:B:157:LEU:H	1.63	0.64
1:B:314:LEU:HD13	1:B:346:PHE:HB2	1.80	0.63
1:B:318:ASP:OD2	1:B:321:ARG:HB3	1.98	0.63
1:B:337:TYR:HB2	1:B:341:PRO:HB3	1.79	0.63
1:B:360:ALA:O	1:B:364:LEU:HG	1.97	0.63
1:A:295:ARG:HH11	1:A:295:ARG:CB	2.12	0.62
1:A:102:GLY:O	1:A:152:ARG:HG2	2.01	0.61
1:A:160:THR:HA	1:A:161:PRO:C	2.25	0.60
1:B:159:ASN:OD1	1:B:162:MET:HA	2.01	0.60
1:B:109:GLU:OE1	1:B:128:LEU:HD13	2.02	0.60
1:A:337:TYR:HB2	1:A:341:PRO:HB3	1.84	0.60
1:B:365:GLY:C	1:B:367:VAL:H	2.10	0.60
1:A:99:VAL:HB	1:A:124:ALA:HB2	1.84	0.59
1:B:120:PHE:CD1	1:B:120:PHE:C	2.80	0.59
1:B:361:LEU:O	1:B:364:LEU:HB2	2.00	0.59
1:B:310:LEU:C	1:B:310:LEU:HD23	2.27	0.59
1:A:333:ALA:HB2	1:A:345:LEU:O	2.01	0.59
1:A:366:ARG:HG2	1:A:366:ARG:HH11	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:MET:HE1	1:B:361:LEU:O	2.03	0.59
1:A:305:GLU:HB3	4:A:533:HOH:O	2.03	0.59
1:B:29:ASN:HA	1:B:329:ALA:HB3	1.83	0.58
1:B:155:ALA:HB2	1:B:187:PHE:HB2	1.85	0.57
1:A:109:GLU:OE1	1:A:130:ARG:NE	2.37	0.57
1:B:194:TYR:HE2	2:B:1510:PLP:HO3	1.51	0.57
1:A:135:PRO:HB3	1:A:300:ARG:HH21	1.69	0.57
1:B:104:GLU:CD	1:B:127:ARG:HH12	2.11	0.57
1:B:160:THR:HA	1:B:161:PRO:C	2.29	0.57
1:A:3:LEU:CD1	1:B:243:ARG:HG3	2.35	0.57
1:A:178:ALA:O	1:A:182:ARG:HG3	2.05	0.57
1:A:238:LYS:HA	1:A:241:MET:HG2	1.87	0.57
1:A:66:LEU:HD22	1:A:70:LEU:CD2	2.32	0.56
1:B:14:ILE:HG23	1:B:15:PHE:N	2.19	0.56
1:B:66:LEU:HD13	1:B:83:VAL:HG21	1.86	0.56
1:B:99:VAL:HG11	1:B:105:VAL:CG2	2.36	0.56
1:B:173:GLU:O	1:B:177:ILE:HG13	2.06	0.56
1:A:135:PRO:HB3	1:A:300:ARG:NH2	2.20	0.56
1:A:248:ARG:HD3	1:A:248:ARG:C	2.30	0.56
1:A:64:PRO:O	1:A:68:GLU:HG3	2.06	0.56
1:A:367:VAL:O	1:A:368:VAL:O	2.24	0.56
1:A:249:GLN:NE2	1:B:13:SER:H	2.02	0.56
1:B:79:GLU:CD	1:B:79:GLU:H	2.14	0.55
1:A:271:ARG:HB2	1:A:272:ARG:NH1	2.22	0.55
1:B:66:LEU:HD22	1:B:70:LEU:HD22	1.88	0.55
1:A:134:THR:C	1:A:136:GLU:H	2.14	0.55
1:B:289:LEU:HD22	1:B:357:LEU:HD13	1.88	0.55
1:B:80:SER:HA	1:B:241:MET:HG3	1.88	0.55
1:B:94:LEU:HD13	1:B:234:ILE:HD13	1.87	0.55
1:B:289:LEU:C	1:B:289:LEU:HD23	2.32	0.54
1:B:109:GLU:HG2	1:B:337:TYR:CD1	2.42	0.54
1:B:111:PHE:CZ	1:B:116:LEU:HD22	2.43	0.54
1:A:366:ARG:HG2	1:A:366:ARG:NH1	2.23	0.54
1:B:77:GLU:HG2	1:B:79:GLU:HG2	1.90	0.54
1:B:238:LYS:HA	1:B:241:MET:HG2	1.89	0.54
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.73	0.54
1:A:3:LEU:HD11	1:B:243:ARG:HG3	1.89	0.54
3:A:520:KMT:H53	1:B:57:TYR:CZ	2.43	0.54
1:A:147:LYS:O	1:A:147:LYS:HG2	2.06	0.54
1:A:365:GLY:C	1:A:367:VAL:H	2.15	0.53
1:B:279:LEU:O	1:B:283:TYR:HD1	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:C	1:A:310:LEU:HD23	2.33	0.53
1:B:359:LEU:O	1:B:363:ARG:HG3	2.09	0.53
1:A:109:GLU:HA	1:A:110:PRO:C	2.33	0.53
1:A:133:LEU:HD13	1:A:138:PHE:CE1	2.44	0.53
1:B:310:LEU:HD23	1:B:310:LEU:O	2.08	0.52
1:A:160:THR:O	1:A:192:GLU:HG2	2.10	0.52
1:A:13:SER:H	1:B:249:GLN:HE22	1.57	0.52
1:A:134:THR:HG23	1:A:137:GLY:O	2.10	0.52
1:A:256:PRO:HA	1:B:228:GLY:O	2.09	0.52
1:B:77:GLU:CG	1:B:79:GLU:HG2	2.40	0.52
1:B:20:GLY:O	1:B:24:ARG:HB2	2.10	0.51
1:B:311:MET:HE2	1:B:345:LEU:HG	1.93	0.51
1:B:268:LYS:HD3	1:B:272:ARG:NH2	2.26	0.51
1:A:120:PHE:C	1:A:120:PHE:CD1	2.89	0.51
1:B:110:PRO:HB2	1:B:336:PHE:HB3	1.91	0.51
1:B:145:LEU:HD22	1:B:180:LEU:CD1	2.41	0.51
1:A:99:VAL:O	1:B:6:ARG:NH2	2.44	0.51
1:A:253:PHE:CZ	3:B:1520:KMT:S1	3.04	0.51
1:A:149:LEU:N	1:A:149:LEU:HD12	2.26	0.51
1:A:196:GLU:OE2	1:A:271:ARG:NH2	2.43	0.51
1:B:9:ALA:O	1:B:11:LYS:N	2.38	0.50
1:A:2:ARG:HH11	1:A:2:ARG:HG2	1.75	0.50
1:B:127:ARG:NH2	1:B:127:ARG:HB2	2.26	0.50
1:B:318:ASP:O	1:B:322:LEU:HD12	2.10	0.50
1:A:209:PHE:H	1:A:209:PHE:HD1	1.59	0.50
1:B:109:GLU:OE2	1:B:337:TYR:HD1	1.93	0.50
1:B:158:LEU:HD11	1:B:169:PHE:CE1	2.46	0.50
1:A:182:ARG:HG2	1:A:213:ARG:HE	1.76	0.50
1:B:366:ARG:O	1:B:367:VAL:HG23	2.11	0.50
1:A:365:GLY:O	1:A:367:VAL:N	2.45	0.50
1:A:110:PRO:HB2	1:A:336:PHE:HB3	1.93	0.49
1:B:28:VAL:HG23	1:B:363:ARG:HH21	1.75	0.49
1:A:60:PRO:HA	1:A:254:SER:HB3	1.95	0.49
1:B:108:LEU:HB2	4:B:1526:HOH:O	2.12	0.49
1:A:209:PHE:CD1	1:A:209:PHE:N	2.81	0.49
1:A:66:LEU:HD13	1:A:83:VAL:CG2	2.39	0.49
1:A:105:VAL:HG23	1:A:124:ALA:HB1	1.95	0.49
1:B:314:LEU:HD13	1:B:346:PHE:CD1	2.47	0.49
1:A:317:TRP:CZ2	1:A:367:VAL:HG12	2.47	0.49
1:B:64:PRO:O	1:B:68:GLU:HG3	2.12	0.49
1:B:120:PHE:C	1:B:120:PHE:HD1	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:VAL:HG23	1:B:153:THR:CG2	2.43	0.49
1:B:314:LEU:N	1:B:314:LEU:HD12	2.28	0.49
1:B:237:PRO:HG2	1:B:240:PHE:HD2	1.77	0.48
1:B:129:VAL:HG12	1:B:129:VAL:O	2.14	0.48
1:A:236:GLY:O	1:A:237:PRO:C	2.56	0.48
1:A:272:ARG:HG2	1:A:272:ARG:HH11	1.79	0.48
1:A:333:ALA:HB2	1:A:345:LEU:HB3	1.96	0.48
1:B:109:GLU:HA	1:B:110:PRO:C	2.39	0.48
1:B:323:VAL:O	1:B:323:VAL:HG22	2.14	0.48
1:A:311:MET:HE2	1:A:345:LEU:HG	1.95	0.48
1:A:4:HIS:CD2	1:B:100:GLY:HA3	2.49	0.48
1:B:169:PHE:CD2	1:B:169:PHE:N	2.81	0.48
1:A:1:MET:CE	1:B:213:ARG:HH11	2.27	0.48
1:B:295:ARG:NE	1:B:301:VAL:HB	2.25	0.48
1:B:309:PHE:O	1:B:350:PHE:HE2	1.97	0.48
1:A:158:LEU:HD22	1:A:169:PHE:CE1	2.46	0.47
1:B:168:VAL:CG2	1:B:305:GLU:HB2	2.43	0.47
1:A:198:TYR:OH	1:A:202:ARG:NH2	2.46	0.47
1:A:281:GLU:CD	1:A:284:ARG:HH12	2.22	0.47
1:B:18:MET:HE3	1:B:329:ALA:HB1	1.96	0.47
1:B:49:ARG:NH1	1:B:265:GLU:OE2	2.36	0.47
1:B:107:VAL:HG12	1:B:108:LEU:O	2.15	0.47
1:B:166:GLY:HA3	1:B:304:PRO:CB	2.45	0.47
1:B:361:LEU:HA	1:B:364:LEU:HD12	1.96	0.47
1:A:289:LEU:HD23	1:A:289:LEU:C	2.39	0.47
1:B:14:ILE:CG2	1:B:15:PHE:N	2.77	0.47
1:B:170:GLY:O	1:B:174:LEU:HD23	2.15	0.47
1:A:363:ARG:O	1:A:367:VAL:HG23	2.15	0.47
1:B:66:LEU:HD22	1:B:70:LEU:CD2	2.45	0.47
1:B:132:ASP:HB2	1:B:139:ARG:HB3	1.97	0.46
1:B:268:LYS:CA	1:B:268:LYS:HE2	2.45	0.46
1:B:314:LEU:CD1	1:B:346:PHE:HB2	2.45	0.46
1:B:160:THR:HA	1:B:162:MET:N	2.31	0.46
1:A:341:PRO:O	1:A:342:PRO:C	2.59	0.46
1:B:295:ARG:O	1:B:298:GLY:N	2.49	0.46
1:A:97:SER:O	1:A:98:LEU:HD23	2.15	0.46
1:A:130:ARG:HE	1:A:130:ARG:HB2	1.61	0.46
1:A:333:ALA:C	1:A:335:ALA:H	2.23	0.46
1:B:268:LYS:HE2	1:B:268:LYS:HA	1.98	0.46
1:B:104:GLU:OE1	1:B:152:ARG:HB2	2.16	0.46
1:A:182:ARG:NH1	1:A:209:PHE:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ALA:O	1:B:94:LEU:HB2	2.16	0.46
1:A:25:LEU:HD22	4:A:531:HOH:O	2.16	0.46
1:A:55:ASP:OD2	1:B:39:PRO:HD2	2.16	0.46
1:A:249:GLN:NE2	1:B:13:SER:OG	2.49	0.46
1:B:109:GLU:O	1:B:131:LEU:HD13	2.16	0.45
1:B:268:LYS:HE2	1:B:268:LYS:N	2.31	0.45
1:A:91:LEU:HD11	1:A:191:ASP:OD2	2.16	0.45
1:B:164:PRO:CB	1:B:347:ARG:HD3	2.46	0.45
1:A:343:LYS:O	1:A:344:ASP:HB2	2.15	0.45
1:B:207:ARG:HD3	4:B:1562:HOH:O	2.16	0.45
1:A:6:ARG:C	1:A:8:GLU:H	2.24	0.45
1:A:104:GLU:HG3	1:A:152:ARG:HB3	1.99	0.45
1:B:320:PHE:HD1	1:B:320:PHE:H	1.59	0.45
1:B:366:ARG:O	1:B:367:VAL:CG2	2.65	0.45
1:B:15:PHE:CE2	1:B:113:ASP:OD2	2.70	0.45
1:A:4:HIS:NE2	1:B:100:GLY:HA3	2.31	0.45
1:B:34:PHE:CD1	1:B:34:PHE:O	2.69	0.45
1:A:134:THR:C	1:A:136:GLU:N	2.76	0.44
1:B:313:GLU:C	1:B:314:LEU:HD12	2.42	0.44
1:B:315:PRO:HA	1:B:344:ASP:OD1	2.16	0.44
1:B:277:GLU:HB2	4:B:1528:HOH:O	2.17	0.44
1:B:329:ALA:O	1:B:330:LEU:HD23	2.18	0.44
1:B:149:LEU:HD21	1:B:186:LEU:HD11	1.99	0.44
1:B:210:ALA:N	1:B:211:PRO:CD	2.81	0.44
1:B:21:LEU:HG	1:B:25:LEU:CD1	2.48	0.44
1:B:133:LEU:HD11	1:B:302:TYR:CE2	2.53	0.44
1:B:193:VAL:HG12	1:B:219:SER:HB3	1.99	0.44
1:B:291:ALA:HB1	1:B:301:VAL:HG11	1.99	0.44
1:A:40:PRO:HA	1:A:41:PRO:HD3	1.91	0.44
1:A:90:ALA:O	1:A:94:LEU:HB2	2.18	0.44
1:A:313:GLU:HA	1:A:344:ASP:O	2.17	0.44
1:B:106:VAL:HG23	1:B:153:THR:HG23	2.00	0.44
1:B:141:ASP:C	1:B:143:SER:N	2.75	0.44
1:A:15:PHE:HB2	1:A:16:PRO:CD	2.48	0.44
1:B:169:PHE:N	1:B:169:PHE:HD2	2.15	0.43
1:B:98:LEU:HD12	1:B:189:ILE:HD11	2.00	0.43
1:A:48:ARG:HG3	1:A:48:ARG:HH11	1.84	0.43
1:A:168:VAL:CG2	1:A:305:GLU:HB2	2.44	0.43
1:B:25:LEU:HD13	1:B:323:VAL:O	2.18	0.43
1:B:60:PRO:HA	1:B:254:SER:HB3	2.01	0.43
1:B:299:LEU:HD11	4:B:1559:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:O	1:A:363:ARG:HG3	2.17	0.43
1:B:63:LEU:O	1:B:64:PRO:C	2.60	0.43
1:B:137:GLY:HA2	1:B:302:TYR:HD2	1.83	0.43
1:B:241:MET:HB2	1:B:242:PRO:HD3	2.01	0.43
1:B:249:GLN:O	1:B:253:PHE:HA	2.19	0.43
1:B:333:ALA:HA	1:B:336:PHE:HD2	1.83	0.43
1:B:366:ARG:C	1:B:367:VAL:HG23	2.44	0.43
1:B:21:LEU:HG	1:B:25:LEU:HD12	2.01	0.43
1:B:87:ALA:O	1:B:90:ALA:N	2.50	0.43
1:B:365:GLY:O	1:B:367:VAL:N	2.49	0.43
1:A:228:GLY:O	1:B:256:PRO:HA	2.18	0.43
1:A:84:THR:HA	1:A:248:ARG:NH2	2.34	0.43
1:A:97:SER:OG	1:A:247:MET:HG3	2.18	0.43
1:B:204:ARG:HE	1:B:208:GLU:CD	2.27	0.43
1:A:272:ARG:HA	1:A:272:ARG:HD3	1.80	0.43
1:B:302:TYR:N	1:B:302:TYR:CD1	2.87	0.43
1:B:87:ALA:O	1:B:90:ALA:HB3	2.19	0.42
1:A:13:SER:H	1:B:249:GLN:NE2	2.17	0.42
1:B:141:ASP:OD2	1:B:143:SER:HB2	2.20	0.42
1:B:159:ASN:O	1:B:162:MET:HA	2.19	0.42
1:A:366:ARG:HD2	1:A:366:ARG:O	2.19	0.42
1:A:164:PRO:HB3	1:A:347:ARG:HD3	2.01	0.42
1:A:29:ASN:O	1:A:352:LYS:HE3	2.19	0.42
1:A:171:GLU:OE1	1:A:204:ARG:NE	2.53	0.42
1:B:268:LYS:HA	1:B:272:ARG:HH21	1.83	0.42
1:A:4:HIS:ND1	1:A:5:PRO:HD2	2.35	0.42
1:A:74:PHE:O	1:A:75:ALA:HB3	2.18	0.42
1:B:167:LEU:HD12	1:B:305:GLU:OE2	2.20	0.42
1:A:18:MET:HE3	1:A:329:ALA:HB1	2.01	0.42
1:A:116:LEU:HB2	1:A:117:PRO:HD3	2.02	0.42
1:B:99:VAL:HG11	1:B:105:VAL:HG23	2.02	0.42
1:B:156:LEU:HD23	1:B:157:LEU:N	2.30	0.42
1:A:272:ARG:NH1	1:A:272:ARG:HG2	2.34	0.42
1:B:81:VAL:HG22	1:B:235:VAL:HG22	2.02	0.42
1:B:154:ARG:NH1	1:B:154:ARG:HG2	2.35	0.42
1:B:194:TYR:HE2	2:B:1510:PLP:O3	2.02	0.42
1:A:193:VAL:HG23	1:A:194:TYR:CD2	2.55	0.41
1:B:30:LEU:N	1:B:30:LEU:HD23	2.35	0.41
1:B:91:LEU:O	1:B:92:TYR:C	2.62	0.41
1:B:127:ARG:HH11	1:B:150:THR:HG23	1.85	0.41
1:B:339:GLU:O	1:B:340:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:OE2	1:A:238:LYS:HD2	2.19	0.41
1:A:111:PHE:CZ	1:A:116:LEU:HD22	2.54	0.41
1:A:112:PHE:HB3	1:A:115:TYR:CZ	2.56	0.41
1:B:365:GLY:C	1:B:367:VAL:N	2.76	0.41
1:B:164:PRO:HB3	1:B:347:ARG:HD3	2.02	0.41
1:A:104:GLU:OE1	1:A:127:ARG:HD3	2.20	0.41
1:A:179:ARG:HG3	1:A:179:ARG:HH11	1.86	0.41
1:A:238:LYS:O	1:A:242:PRO:HD3	2.19	0.41
1:B:6:ARG:C	1:B:8:GLU:H	2.29	0.41
1:A:171:GLU:O	1:A:175:GLU:HG3	2.20	0.41
1:A:256:PRO:HB2	1:A:259:LEU:HB2	2.01	0.41
1:B:114:VAL:CG1	1:B:118:ASP:OD2	2.60	0.41
1:B:319:ALA:O	1:B:322:LEU:HB2	2.20	0.41
1:A:76:VAL:CG1	1:A:207:ARG:NH2	2.83	0.41
1:A:367:VAL:O	1:A:367:VAL:HG12	2.20	0.41
1:B:285:ARG:C	1:B:287:ARG:N	2.79	0.41
1:B:8:GLU:OE2	1:B:120:PHE:HZ	2.04	0.41
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.95	0.41
1:A:99:VAL:HG11	1:A:105:VAL:CG2	2.46	0.41
1:A:104:GLU:HB2	1:A:153:THR:HA	2.03	0.41
1:A:281:GLU:OE1	1:A:284:ARG:NH1	2.54	0.41
1:B:149:LEU:CD2	1:B:186:LEU:HD11	2.50	0.41
1:B:252:SER:O	1:B:254:SER:N	2.54	0.41
1:B:348:PHE:O	1:B:349:ALA:HB2	2.21	0.41
1:B:24:ARG:HE	1:B:24:ARG:HB3	1.66	0.41
1:A:100:GLY:HA3	1:B:4:HIS:NE2	2.36	0.40
1:B:30:LEU:HD22	1:B:352:LYS:HG3	2.03	0.40
1:B:284:ARG:O	1:B:285:ARG:C	2.65	0.40
1:B:284:ARG:O	1:B:287:ARG:HB3	2.21	0.40
1:B:327:ARG:HA	1:B:327:ARG:HD3	1.85	0.40
1:B:164:PRO:HB2	1:B:347:ARG:CD	2.51	0.40
1:B:362:GLU:C	1:B:364:LEU:N	2.79	0.40
1:A:181:ALA:HB1	1:A:213:ARG:HD2	2.03	0.40
1:A:249:GLN:NE2	1:B:13:SER:CB	2.84	0.40
1:A:93:VAL:HG13	1:A:247:MET:HB3	2.02	0.40
1:A:249:GLN:HA	1:A:253:PHE:HA	2.02	0.40
1:B:193:VAL:HG23	1:B:194:TYR:CD2	2.56	0.40
1:A:89:GLU:HA	1:B:251:THR:O	2.22	0.40
1:B:40:PRO:HA	1:B:41:PRO:HD3	1.88	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1557:HOH:O	4:B:1557:HOH:O[4_555]	1.94	0.26

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	366/381 (96%)	329 (90%)	27 (7%)	10 (3%)	4	7
1	B	365/381 (96%)	308 (84%)	47 (13%)	10 (3%)	4	7
All	All	731/762 (96%)	637 (87%)	74 (10%)	20 (3%)	4	7

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	B	349	ALA
1	A	57	TYR
1	A	124	ALA
1	A	366	ARG
1	B	129	VAL
1	A	253	PHE
1	A	342	PRO
1	B	7	THR
1	B	10	ALA
1	B	113	ASP
1	B	253	PHE
1	A	115	TYR
1	A	153	THR
1	B	310	LEU
1	B	366	ARG
1	A	334	SER
1	B	285	ARG
1	B	342	PRO
1	A	135	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	294/302 (97%)	271 (92%)	23 (8%)	11	26
1	B	293/302 (97%)	274 (94%)	19 (6%)	15	35
All	All	587/604 (97%)	545 (93%)	42 (7%)	13	30

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	60	PRO
1	A	66	LEU
1	A	70	LEU
1	A	94	LEU
1	A	105	VAL
1	A	127	ARG
1	A	134	THR
1	A	136	GLU
1	A	145	LEU
1	A	164	PRO
1	A	201	GLU
1	A	248	ARG
1	A	249	GLN
1	A	269	LEU
1	A	290	LEU
1	A	295	ARG
1	A	310	LEU
1	A	343	LYS
1	A	355	GLU
1	A	359	LEU
1	A	363	ARG
1	A	366	ARG
1	B	1	MET
1	B	18	MET
1	B	28	VAL
1	B	66	LEU

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Mol	Chain	Res	Type
1	B	70	LEU
1	B	79	GLU
1	B	94	LEU
1	B	120	PHE
1	B	145	LEU
1	B	158	LEU
1	B	164	PRO
1	B	239	GLU
1	B	259	LEU
1	B	269	LEU
1	B	289	LEU
1	B	308	TYR
1	B	310	LEU
1	B	342	PRO
1	B	359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	249	GLN
1	B	37	ASN
1	B	249	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](#)

4 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
2	PLP	B	1510	1	15,15,16	1.47	4 (26%)	21,22,23	1.32	2 (9%)
2	PLP	A	510	1	15,15,16	1.35	1 (6%)	21,22,23	1.45	2 (9%)
3	KMT	B	1520	-	8,8,8	2.82	4 (50%)	7,9,9	2.73	2 (28%)
3	KMT	A	520	-	8,8,8	2.81	4 (50%)	7,9,9	3.01	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	1510	1	-	1/6/6/8	0/1/1/1
2	PLP	A	510	1	-	2/6/6/8	0/1/1/1
3	KMT	B	1520	-	-	4/8/8/8	-
3	KMT	A	520	-	-	5/8/8/8	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1520	KMT	O1-C1	-5.27	1.16	1.30
3	A	520	KMT	O1-C1	-5.17	1.16	1.30
3	A	520	KMT	C3-C2	-3.59	1.47	1.51
3	A	520	KMT	C2-C1	-3.51	1.48	1.53
3	B	1520	KMT	C3-C2	-3.35	1.47	1.51
3	B	1520	KMT	O2-C1	3.26	1.30	1.22
3	B	1520	KMT	C2-C1	-3.15	1.48	1.53
2	A	510	PLP	C3-C2	-3.02	1.37	1.41
2	B	1510	PLP	C2A-C2	2.92	1.55	1.50
3	A	520	KMT	O2-C1	2.76	1.29	1.22
2	B	1510	PLP	C3-C2	-2.59	1.38	1.41
2	B	1510	PLP	P-O2P	2.15	1.62	1.54
2	B	1510	PLP	C4A-C4	2.06	1.55	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	520	KMT	O2-C1-C2	-6.73	113.44	121.81
3	B	1520	KMT	O2-C1-C2	-6.16	114.15	121.81
2	A	510	PLP	O4P-C5A-C5	3.49	115.90	109.36
2	A	510	PLP	O3P-P-O4P	3.26	115.16	106.67
2	B	1510	PLP	C6-C5-C4	2.64	120.26	118.10
3	A	520	KMT	C3-C2-C1	2.46	120.04	115.86
3	B	1520	KMT	C3-C2-C1	2.30	119.78	115.86
2	B	1510	PLP	O4P-C5A-C5	2.28	113.63	109.36
3	A	520	KMT	O5-C2-C1	-2.01	116.80	119.67

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	510	PLP	C5A-O4P-P-O2P
2	A	510	PLP	C5A-O4P-P-O3P
3	A	520	KMT	O1-C1-C2-C3
3	B	1520	KMT	O1-C1-C2-C3
3	B	1520	KMT	O2-C1-C2-O5
3	B	1520	KMT	O2-C1-C2-C3
3	B	1520	KMT	O5-C2-C3-C4
3	A	520	KMT	O5-C2-C3-C4
3	A	520	KMT	O2-C1-C2-O5
2	B	1510	PLP	C5A-O4P-P-O3P
3	A	520	KMT	O2-C1-C2-C3
3	A	520	KMT	C1-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1510	PLP	2	0
3	B	1520	KMT	1	0
3	A	520	KMT	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	368/381 (96%)	-0.15	6 (1%) 70 66	14, 36, 61, 71	0
1	B	367/381 (96%)	0.14	9 (2%) 58 52	10, 47, 69, 78	0
All	All	735/762 (96%)	-0.01	15 (2%) 65 60	10, 40, 67, 78	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	VAL	4.0
1	B	318	ASP	3.6
1	A	183	ALA	3.5
1	B	344	ASP	2.5
1	B	143	SER	2.4
1	B	346	PHE	2.3
1	B	27	ALA	2.3
1	B	323	VAL	2.3
1	A	152	ARG	2.2
1	B	2	ARG	2.2
1	B	340	ASP	2.1
1	A	343	LYS	2.1
1	B	132	ASP	2.1
1	A	100	GLY	2.1
1	A	341	PRO	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	KMT	B	1520	9/9	0.91	0.08	39,43,45,45	0
3	KMT	A	520	9/9	0.95	0.08	34,35,36,36	0
2	PLP	B	1510	15/16	0.97	0.06	22,27,29,29	0
2	PLP	A	510	15/16	0.98	0.05	17,19,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.