



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:37 AM UTC

PDB ID : 3DU4 / pdb_00003du4
Title : Crystal structure of 7-keto-8-aminopelargonic acid bound 7,8-diaminopelargonic acid synthase in bacillus subtilis
Authors : Dey, S.; Sacchettini, J.C.
Deposited on : 2008-07-16
Resolution : 2.20 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

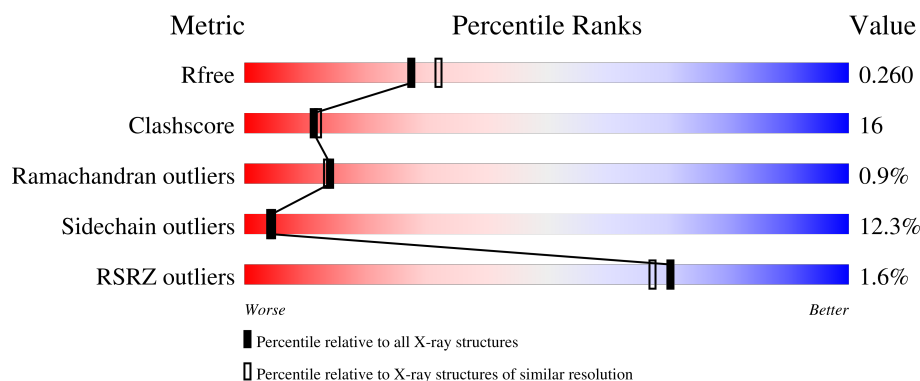
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 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	448	2% 68% 26% 5%
1	B	448	% 65% 27% 7%

2 Entry composition [i](#)

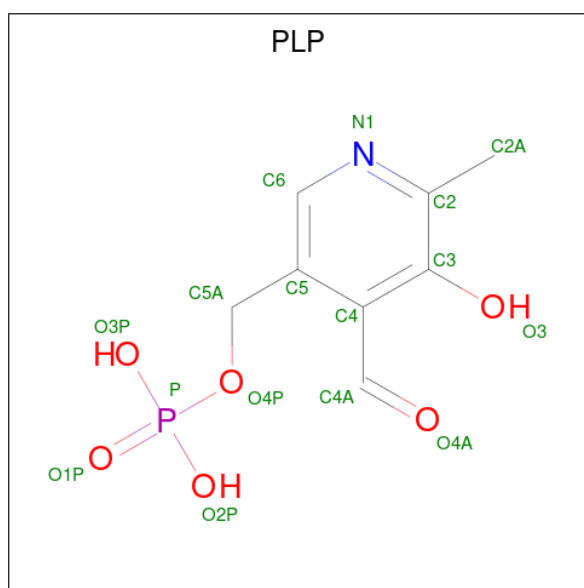
There are 4 unique types of molecules in this entry. The entry contains 7355 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosylmethionine-8-amino-7-oxononanoate aminotransferase.

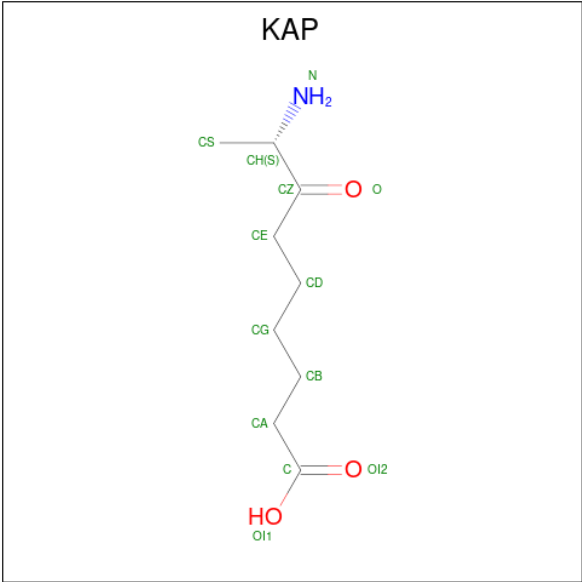
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3519	2246	582	667	24			
1	B	448	Total	C	N	O	S	0	0	0
			3519	2246	582	667	24			

- 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 7-KETO-8-AMINOPELARGONIC ACID (CCD ID: KAP) (formula: $C_9H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		

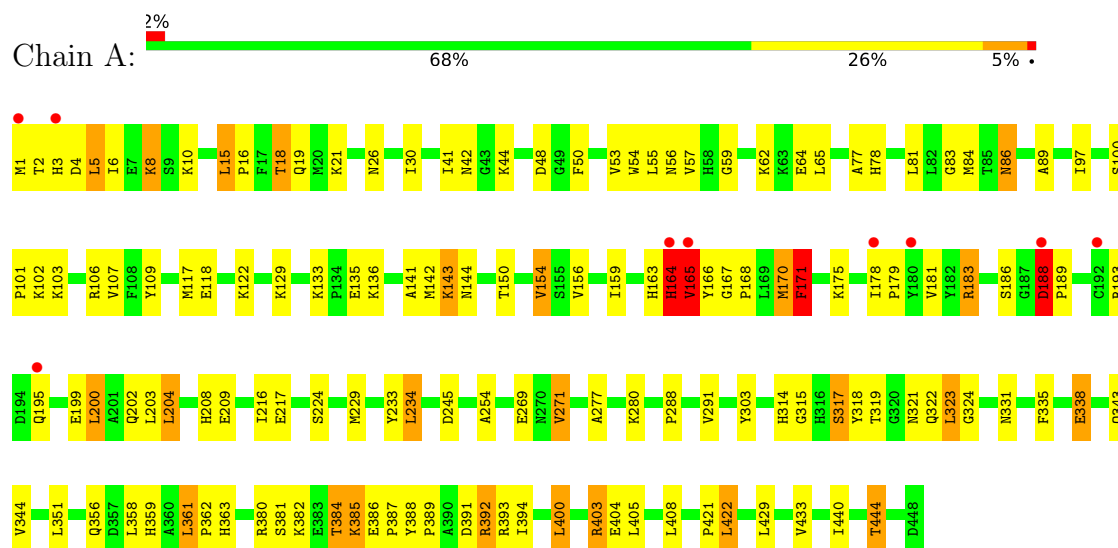
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	141	Total	O	0	0
			141	141		

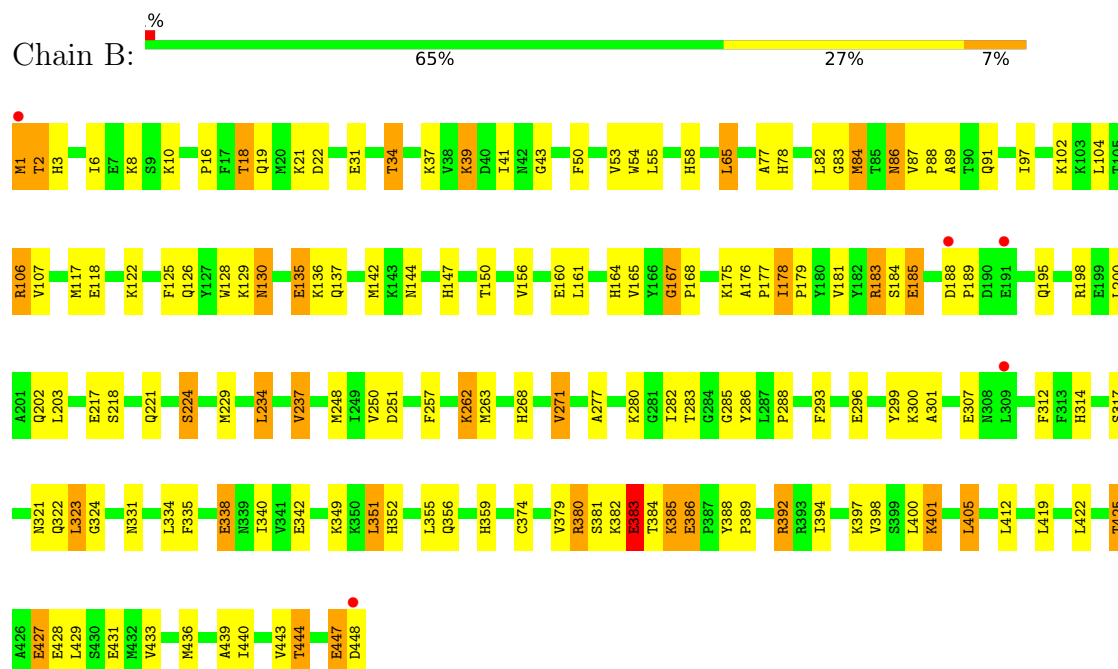
3 Residue-property plots

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: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.69Å 105.13Å 75.06Å 90.00° 105.19° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.20) 99.3 (30.00-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.260 0.200 , 0.260	Depositor DCC
R_{free} test set	2200 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7355	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: KAP, CSX, 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	0.63	0/3587	1.00	10/4841 (0.2%)
1	B	0.66	0/3587	0.96	4/4841 (0.1%)
All	All	0.65	0/7174	0.98	14/9682 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	VAL	N-CA-C	-14.24	95.47	111.00
1	B	2	THR	N-CA-C	-7.58	103.12	114.64
1	A	15	LEU	CA-C-N	7.08	126.84	119.76
1	A	15	LEU	C-N-CA	7.08	126.84	119.76
1	A	171	PHE	CB-CA-C	6.25	122.86	110.42
1	A	188	ASP	CA-C-N	6.19	125.59	118.85
1	A	188	ASP	C-N-CA	6.19	125.59	118.85
1	A	361	LEU	CA-C-N	5.86	125.72	119.28
1	A	361	LEU	C-N-CA	5.86	125.72	119.28
1	B	130	ASN	N-CA-C	5.73	118.27	111.33
1	A	181	VAL	N-CA-C	5.47	116.20	110.62
1	A	5	LEU	N-CA-C	-5.28	105.53	111.28
1	B	167	GLY	O-C-N	5.20	122.94	121.07
1	B	102	LYS	N-CA-C	5.01	118.16	111.75

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	171	PHE	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	HIS	Peptide
1	A	170	MET	Peptide

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	3519	0	3493	118	0
1	B	3519	0	3493	128	0
2	A	15	0	7	1	0
2	B	15	0	7	0	0
3	A	13	0	16	1	0
3	B	13	0	16	1	0
4	A	120	0	0	4	0
4	B	141	0	0	4	0
All	All	7355	0	7032	227	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 16.

All (227) 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:A:141:ALA:HB2	1:A:156:VAL:CG2	1.82	1.08
1:B:142:MET:HB3	1:B:178:ILE:HD11	1.37	1.06
1:A:141:ALA:HB2	1:A:156:VAL:HG22	1.32	1.05
1:B:425:THR:CG2	1:B:427:GLU:HG2	1.90	1.01
1:A:2:THR:HG21	1:A:42:ASN:HD21	1.24	1.00
1:A:117:MET:HE3	1:A:277:ALA:HB3	1.43	1.00
1:B:178:ILE:HG22	1:B:179:PRO:HD2	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:MET:HE3	1:B:277:ALA:CB	1.95	0.97
1:B:117:MET:HE3	1:B:277:ALA:HB3	1.47	0.95
1:B:142:MET:CB	1:B:178:ILE:HD11	1.98	0.94
1:A:150:THR:HG22	1:B:118:GLU:HG2	1.50	0.93
1:A:117:MET:HE3	1:A:277:ALA:CB	1.98	0.92
1:B:117:MET:CE	1:B:277:ALA:HB2	1.99	0.92
1:B:142:MET:HB3	1:B:178:ILE:CD1	1.99	0.92
1:A:117:MET:CE	1:A:277:ALA:HB2	2.05	0.86
1:B:381:SER:OG	1:B:383:GLU:HG3	1.75	0.86
1:A:117:MET:CE	1:A:277:ALA:CB	2.56	0.84
1:B:117:MET:HE2	1:B:277:ALA:HB2	1.59	0.84
1:B:178:ILE:HG22	1:B:179:PRO:CD	2.07	0.83
1:A:159:ILE:H	1:A:163:HIS:HD2	1.22	0.83
1:A:234:LEU:HD13	1:A:271:VAL:HG11	1.61	0.83
1:A:117:MET:HE2	1:A:277:ALA:HB2	1.57	0.82
1:A:141:ALA:CB	1:A:156:VAL:HG22	2.09	0.82
1:B:117:MET:CE	1:B:277:ALA:CB	2.57	0.82
1:B:1:MET:HE2	1:B:3:HIS:H	1.46	0.81
1:A:164:HIS:CG	1:A:164:HIS:O	2.34	0.81
1:B:16:PRO:O	1:B:18:THR:HG22	1.82	0.79
1:A:159:ILE:H	1:A:163:HIS:CD2	2.00	0.78
1:B:425:THR:HG21	1:B:427:GLU:HG2	1.67	0.77
1:A:183:ARG:CB	1:A:183:ARG:HH11	1.99	0.76
1:A:122:LYS:HE2	1:A:314:HIS:ND1	2.01	0.76
1:B:425:THR:HG22	1:B:428:GLU:H	1.51	0.76
1:B:443:VAL:HG13	1:B:448:ASP:OD1	1.88	0.74
1:B:39:LYS:HD3	1:B:43:GLY:HA2	1.68	0.74
1:A:19:GLN:HE21	1:A:21:LYS:H	1.34	0.74
1:A:363:HIS:CD2	1:A:444:THR:HG23	2.23	0.72
1:A:2:THR:HG21	1:A:42:ASN:ND2	2.03	0.72
1:A:165:VAL:HG12	1:B:129:LYS:HD3	1.71	0.72
1:A:209:GLU:HB2	4:A:563:HOH:O	1.89	0.70
1:B:184:SER:OG	1:B:185:GLU:N	2.22	0.70
1:A:440:ILE:O	1:A:444:THR:HB	1.90	0.69
1:A:168:PRO:HG2	1:B:125:PHE:HZ	1.57	0.69
1:B:440:ILE:O	1:B:444:THR:HB	1.92	0.69
1:B:34:THR:CG2	4:B:500:HOH:O	2.40	0.68
1:A:141:ALA:HB2	1:A:156:VAL:HG23	1.71	0.67
1:B:16:PRO:O	1:B:18:THR:CG2	2.43	0.66
1:A:363:HIS:HB2	1:A:444:THR:HG21	1.78	0.66
1:B:1:MET:HE2	1:B:3:HIS:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:THR:HG23	4:B:500:HOH:O	1.97	0.65
1:A:183:ARG:HH11	1:A:183:ARG:CG	2.10	0.64
1:B:86:ASN:ND2	1:B:88:PRO:HD2	2.12	0.64
1:B:144:ASN:HB3	1:B:224:SER:OG	1.97	0.64
1:B:86:ASN:HD22	1:B:88:PRO:HD2	1.62	0.63
1:A:2:THR:HG22	1:A:6:ILE:HD12	1.80	0.63
1:B:19:GLN:HE21	1:B:21:LYS:H	1.47	0.63
1:B:447:GLU:O	1:B:448:ASP:C	2.40	0.62
1:A:83:GLY:H	1:B:18:THR:HG21	1.63	0.62
1:B:178:ILE:HD12	1:B:221:GLN:NE2	2.14	0.62
1:A:195:GLN:O	1:A:199:GLU:HG3	2.00	0.62
1:A:164:HIS:O	1:A:164:HIS:CD2	2.54	0.61
1:A:109:TYR:HB2	1:A:319:THR:HG23	1.81	0.61
1:A:288:PRO:HG2	1:B:288:PRO:HG2	1.82	0.61
1:A:150:THR:O	1:A:154:VAL:HG13	2.00	0.60
1:B:321:ASN:HD22	1:B:324:GLY:H	1.51	0.59
1:B:401:LYS:HA	1:B:401:LYS:HE3	1.83	0.59
1:A:183:ARG:HH11	1:A:183:ARG:HB3	1.68	0.58
1:A:200:LEU:HD22	1:A:204:LEU:HD22	1.84	0.58
1:B:389:PRO:HD2	1:B:392:ARG:HD2	1.85	0.58
1:A:18:THR:HG21	1:B:83:GLY:H	1.68	0.58
1:A:118:GLU:HG2	1:B:150:THR:HA	1.85	0.58
1:B:234:LEU:HD13	1:B:271:VAL:HG11	1.84	0.58
1:B:237:VAL:CG2	1:B:248:MET:HE3	2.34	0.58
1:A:141:ALA:HB3	1:A:175:LYS:NZ	2.19	0.57
1:A:150:THR:CG2	1:B:118:GLU:HG2	2.27	0.57
1:A:86:ASN:ND2	1:A:89:ALA:H	2.04	0.56
1:B:338:GLU:HB3	1:B:340:ILE:HG12	1.88	0.56
1:B:397:LYS:HD3	1:B:448:ASP:HB2	1.87	0.56
1:A:166:TYR:OH	1:B:126:GLN:NE2	2.36	0.56
1:A:204:LEU:O	1:A:208:HIS:HB3	2.06	0.56
1:B:167:GLY:N	1:B:168:PRO:CD	2.68	0.55
1:B:181:VAL:O	1:B:184:SER:HB3	2.06	0.55
1:B:334:LEU:O	1:B:338:GLU:HB2	2.06	0.55
1:B:312:PHE:CE2	1:B:314:HIS:HB3	2.42	0.55
1:A:56:ASN:HD21	1:A:59:GLY:H	1.55	0.55
1:A:384:THR:O	1:A:385:LYS:HG2	2.07	0.55
1:A:4:ASP:HB2	1:A:8:LYS:NZ	2.23	0.54
1:A:315:GLY:HA3	1:B:16:PRO:HB2	1.89	0.54
1:B:425:THR:HG23	1:B:427:GLU:HG2	1.87	0.54
1:A:318:TYR:OH	1:B:285:GLY:HA2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HB3	1:A:16:PRO:HD2	1.91	0.53
1:A:303:TYR:HA	1:B:19:GLN:HE22	1.74	0.53
1:A:30:ILE:CG1	1:B:84:MET:HE3	2.39	0.53
1:A:141:ALA:HB3	1:A:175:LYS:HZ1	1.73	0.52
1:A:217:GLU:O	1:A:229:MET:HE1	2.09	0.52
1:B:178:ILE:CD1	1:B:221:GLN:NE2	2.72	0.52
1:A:254:ALA:HB2	2:A:450:PLP:O3	2.10	0.52
1:A:19:GLN:NE2	1:A:21:LYS:H	2.07	0.52
1:B:384:THR:HB	1:B:386:GLU:H	1.75	0.51
1:A:321:ASN:HD22	1:A:324:GLY:H	1.59	0.51
1:A:386:GLU:HG2	1:A:387:PRO:HD2	1.92	0.51
1:A:77:ALA:HA	1:A:323:LEU:HD13	1.91	0.51
1:A:6:ILE:O	1:A:10:LYS:HG3	2.11	0.51
1:A:388:TYR:CG	1:A:394:ILE:HG13	2.46	0.51
1:A:16:PRO:O	1:A:18:THR:HG23	2.11	0.51
1:B:195:GLN:OE1	1:B:198:ARG:NH2	2.28	0.50
1:B:381:SER:O	1:B:385:LYS:N	2.42	0.50
1:A:429:LEU:O	1:A:433:VAL:HG23	2.10	0.50
1:A:315:GLY:HA3	1:B:16:PRO:CB	2.42	0.50
1:A:56:ASN:HD21	1:A:59:GLY:N	2.10	0.50
1:A:107:VAL:HG13	1:A:291:VAL:HG13	1.93	0.50
1:A:165:VAL:HG11	1:B:126:GLN:HG3	1.93	0.50
1:B:218:SER:HB2	1:B:250:VAL:CG1	2.41	0.50
1:B:296:GLU:O	1:B:300:LYS:HG2	2.12	0.50
1:B:183:ARG:HG3	1:B:183:ARG:HH11	1.77	0.49
1:A:81:LEU:HA	1:A:84:MET:O	2.11	0.49
1:B:118:GLU:O	1:B:122:LYS:HG3	2.12	0.49
1:A:142:MET:HG3	1:A:216:ILE:HD12	1.95	0.49
1:A:164:HIS:HA	1:A:167:GLY:H	1.77	0.49
1:B:58:HIS:NE2	1:B:331:ASN:ND2	2.61	0.49
1:A:381:SER:O	1:A:385:LYS:HA	2.13	0.49
1:B:142:MET:HB2	1:B:178:ILE:HD11	1.86	0.49
1:B:349:LYS:O	1:B:352:HIS:HB3	2.13	0.49
1:B:135:GLU:CD	1:B:135:GLU:H	2.21	0.48
1:B:394:ILE:O	1:B:398:VAL:HG23	2.14	0.48
1:B:389:PRO:O	1:B:392:ARG:HG2	2.13	0.48
1:B:384:THR:HG21	1:B:386:GLU:HB3	1.95	0.48
1:A:62:LYS:HE3	1:A:64:GLU:OE1	2.13	0.48
1:A:78:HIS:CE1	1:A:318:TYR:HA	2.48	0.48
1:A:386:GLU:CG	1:A:387:PRO:HD2	2.44	0.48
1:B:359:HIS:O	1:B:382:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ARG:HB3	1:B:388:TYR:CD2	2.49	0.48
1:B:392:ARG:HE	1:B:392:ARG:HB3	1.53	0.47
1:A:102:LYS:HG3	1:A:103:LYS:N	2.30	0.47
1:B:321:ASN:ND2	1:B:324:GLY:H	2.12	0.47
1:A:54:TRP:CD1	1:A:54:TRP:N	2.83	0.47
1:A:183:ARG:HB3	1:A:183:ARG:NH1	2.28	0.47
1:B:183:ARG:HH11	1:B:183:ARG:CG	2.28	0.47
1:B:142:MET:HB3	1:B:178:ILE:CG1	2.44	0.46
1:A:30:ILE:HG12	1:B:84:MET:HE3	1.97	0.46
3:A:451:KAP:HS1	1:B:82:LEU:HD21	1.96	0.46
1:A:4:ASP:HB2	1:A:8:LYS:HZ1	1.80	0.46
1:A:338:GLU:O	1:A:343:GLN:NE2	2.46	0.46
1:A:144:ASN:HB3	1:A:224:SER:OG	2.15	0.46
1:A:344:VAL:HG21	1:A:422:LEU:HG	1.96	0.46
1:B:217:GLU:O	1:B:229:MET:HE1	2.16	0.46
1:B:401:LYS:HG2	1:B:439:ALA:HA	1.98	0.45
1:B:444:THR:CG2	4:B:537:HOH:O	2.64	0.45
1:A:2:THR:HG23	1:A:41:ILE:CD1	2.47	0.45
1:A:384:THR:C	1:A:385:LYS:HG2	2.41	0.45
1:A:53:VAL:HG12	1:A:53:VAL:O	2.16	0.45
1:A:315:GLY:O	3:B:451:KAP:N	2.45	0.45
1:A:393:ARG:HD2	4:A:500:HOH:O	2.16	0.45
1:B:356:GLN:O	1:B:359:HIS:HB2	2.16	0.45
1:A:56:ASN:HD21	1:A:59:GLY:CA	2.30	0.45
1:B:86:ASN:HD22	1:B:86:ASN:C	2.25	0.45
1:A:331:ASN:HD21	1:A:335:PHE:HE2	1.63	0.45
1:A:321:ASN:ND2	1:A:324:GLY:H	2.15	0.45
1:B:384:THR:CG2	1:B:386:GLU:HB3	2.47	0.45
1:A:234:LEU:HD13	1:A:271:VAL:CG1	2.39	0.45
1:A:361:LEU:HA	1:A:362:PRO:HD3	1.86	0.45
1:B:282:ILE:HG23	1:B:283:THR:HG23	1.98	0.45
1:A:48:ASP:O	1:A:421:PRO:HD3	2.18	0.44
1:B:1:MET:HE3	1:B:1:MET:HB2	1.90	0.44
1:B:1:MET:HE2	1:B:2:THR:H	1.82	0.44
1:B:2:THR:HB	1:B:41:ILE:HD12	2.00	0.44
1:B:128:TRP:CD2	1:B:136:LYS:HD2	2.52	0.44
1:B:19:GLN:O	1:B:22:ASP:HB2	2.17	0.44
1:B:147:HIS:HD2	1:B:251:ASP:OD2	2.00	0.44
1:B:6:ILE:O	1:B:10:LYS:HG3	2.18	0.43
1:B:188:ASP:HA	1:B:189:PRO:HD3	1.85	0.43
1:B:86:ASN:ND2	1:B:89:ALA:H	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:HIS:HB2	1:A:444:THR:CG2	2.47	0.43
1:A:391:ASP:OD2	1:A:391:ASP:C	2.62	0.43
1:A:26:ASN:O	1:A:403:ARG:NH2	2.51	0.43
1:B:77:ALA:HA	1:B:323:LEU:HD13	2.00	0.43
1:A:78:HIS:HA	1:A:322:GLN:OE1	2.19	0.43
1:A:389:PRO:HD2	1:A:392:ARG:HD2	1.99	0.43
1:A:57:VAL:HG13	1:A:422:LEU:HD22	2.00	0.43
1:B:104:LEU:HB3	1:B:293:PHE:HB3	2.00	0.43
1:A:16:PRO:O	1:A:18:THR:CG2	2.67	0.43
1:B:54:TRP:CD1	1:B:54:TRP:N	2.87	0.43
1:B:176:ALA:HA	1:B:177:PRO:HD3	1.82	0.43
1:A:56:ASN:ND2	1:A:59:GLY:H	2.16	0.43
1:B:160:GLU:HB2	1:B:164:HIS:HB2	1.99	0.43
1:B:257:PHE:CZ	1:B:282:ILE:HG13	2.54	0.43
1:A:118:GLU:O	1:A:122:LYS:HG3	2.19	0.42
1:A:178:ILE:HD13	1:A:233:TYR:CE1	2.54	0.42
1:B:427:GLU:O	1:B:431:GLU:HG3	2.19	0.42
1:B:87:VAL:O	1:B:91:GLN:HG3	2.19	0.42
1:B:351:LEU:HD22	1:B:355:LEU:HG	2.01	0.42
1:A:408:LEU:HD13	1:B:84:MET:HE1	2.01	0.42
1:A:136:LYS:HE3	4:A:518:HOH:O	2.19	0.42
1:B:97:ILE:HD11	1:B:107:VAL:HG23	2.02	0.42
1:A:1:MET:HE3	1:A:3:HIS:H	1.84	0.42
1:B:106:ARG:HG2	1:B:299:TYR:CD1	2.55	0.42
1:B:388:TYR:HE2	1:B:447:GLU:HB3	1.85	0.42
1:A:44:LYS:NZ	1:A:404:GLU:HA	2.35	0.41
1:A:183:ARG:HH11	1:A:183:ARG:HG3	1.84	0.41
1:B:1:MET:CE	1:B:2:THR:H	2.33	0.41
1:A:118:GLU:HG2	1:B:150:THR:HG22	2.02	0.41
1:B:78:HIS:HA	1:B:322:GLN:OE1	2.19	0.41
1:A:100:SER:O	1:A:101:PRO:C	2.63	0.41
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.89	0.41
1:B:130:ASN:ND2	1:B:301:ALA:O	2.53	0.41
1:B:444:THR:HG21	4:B:537:HOH:O	2.19	0.41
1:A:163:HIS:O	1:A:164:HIS:HB3	2.21	0.41
1:A:97:ILE:HD11	1:A:107:VAL:HG23	2.03	0.41
1:B:178:ILE:HD12	1:B:221:GLN:CD	2.46	0.41
1:B:436:MET:O	1:B:440:ILE:HG13	2.19	0.41
1:A:317:SER:HB2	1:B:55:LEU:HD23	2.02	0.41
1:B:65:LEU:HD23	1:B:286:TYR:CE1	2.55	0.41
1:A:136:LYS:CE	4:A:518:HOH:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LYS:HD3	1:B:175:LYS:HA	1.88	0.41
1:B:262:LYS:HG2	1:B:268:HIS:CE1	2.56	0.41
1:B:335:PHE:HA	1:B:340:ILE:HG13	2.02	0.41
1:B:54:TRP:CG	1:B:419:LEU:HD22	2.55	0.41
1:B:380:ARG:HG3	1:B:386:GLU:HG2	2.02	0.41
1:A:1:MET:HB3	1:A:4:ASP:OD2	2.21	0.40
1:B:380:ARG:HD3	1:B:386:GLU:OE2	2.21	0.40
1:B:257:PHE:N	1:B:263:MET:O	2.53	0.40
1:A:178:ILE:HG23	1:A:179:PRO:HD2	2.03	0.40
1:B:401:LYS:HG3	1:B:405:LEU:HD22	2.02	0.40
1:B:429:LEU:O	1:B:433:VAL:HG23	2.21	0.40
1:A:188:ASP:HA	1:A:189:PRO:HD3	1.86	0.40
1:A:193:ARG:HG3	1:A:233:TYR:HB2	2.04	0.40
1:A:86:ASN:HD21	1:A:89:ALA:H	1.70	0.40
1:B:296:GLU:HG3	1:B:300:LYS:HE3	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	445/448 (99%)	415 (93%)	26 (6%)	4 (1%)	14	14
1	B	445/448 (99%)	419 (94%)	22 (5%)	4 (1%)	14	14
All	All	890/896 (99%)	834 (94%)	48 (5%)	8 (1%)	14	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	PHE
1	A	186	SER
1	A	280	LYS

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Mol	Chain	Res	Type
1	B	447	GLU
1	B	280	LYS
1	A	143	LYS
1	B	383	GLU
1	B	53	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	377/377 (100%)	333 (88%)	44 (12%)	5	5
1	B	377/377 (100%)	328 (87%)	49 (13%)	4	3
All	All	754/754 (100%)	661 (88%)	93 (12%)	4	4

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	8	LYS
1	A	18	THR
1	A	50	PHE
1	A	55	LEU
1	A	65	LEU
1	A	86	ASN
1	A	106	ARG
1	A	129	LYS
1	A	133	LYS
1	A	135	GLU
1	A	143	LYS
1	A	154	VAL
1	A	164	HIS
1	A	165	VAL
1	A	170	MET
1	A	171	PHE
1	A	183	ARG

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Mol	Chain	Res	Type
1	A	188	ASP
1	A	200	LEU
1	A	202	GLN
1	A	203	LEU
1	A	204	LEU
1	A	234	LEU
1	A	245	ASP
1	A	269	GLU
1	A	271	VAL
1	A	317	SER
1	A	323	LEU
1	A	338	GLU
1	A	351	LEU
1	A	356	GLN
1	A	358	LEU
1	A	359	HIS
1	A	380	ARG
1	A	382	LYS
1	A	384	THR
1	A	385	LYS
1	A	392	ARG
1	A	400	LEU
1	A	403	ARG
1	A	405	LEU
1	A	422	LEU
1	A	444	THR
1	B	1	MET
1	B	8	LYS
1	B	18	THR
1	B	31	GLU
1	B	34	THR
1	B	37	LYS
1	B	39	LYS
1	B	50	PHE
1	B	65	LEU
1	B	84	MET
1	B	86	ASN
1	B	106	ARG
1	B	135	GLU
1	B	137	GLN
1	B	156	VAL
1	B	161	LEU

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Mol	Chain	Res	Type
1	B	165	VAL
1	B	178	ILE
1	B	183	ARG
1	B	185	GLU
1	B	200	LEU
1	B	202	GLN
1	B	203	LEU
1	B	224	SER
1	B	234	LEU
1	B	237	VAL
1	B	262	LYS
1	B	271	VAL
1	B	307	GLU
1	B	317	SER
1	B	323	LEU
1	B	338	GLU
1	B	342	GLU
1	B	351	LEU
1	B	374	CYS
1	B	379	VAL
1	B	380	ARG
1	B	383	GLU
1	B	385	LYS
1	B	386	GLU
1	B	392	ARG
1	B	400	LEU
1	B	401	LYS
1	B	405	LEU
1	B	412	LEU
1	B	422	LEU
1	B	425	THR
1	B	427	GLU
1	B	444	THR

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

Mol	Chain	Res	Type
1	A	19	GLN
1	A	42	ASN
1	A	56	ASN
1	A	86	ASN
1	A	91	GLN

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Mol	Chain	Res	Type
1	A	137	GLN
1	A	144	ASN
1	A	163	HIS
1	A	164	HIS
1	A	202	GLN
1	A	208	HIS
1	A	268	HIS
1	A	321	ASN
1	A	331	ASN
1	B	19	GLN
1	B	42	ASN
1	B	86	ASN
1	B	91	GLN
1	B	126	GLN
1	B	147	HIS
1	B	221	GLN
1	B	308	ASN
1	B	321	ASN
1	B	331	ASN
1	B	356	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSX	A	196	1	3,6,7	0.66	0	1,6,8	0.23	0
1	CSX	B	196	1	3,6,7	0.67	0	1,6,8	0.86	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
1	CSX	A	196	1	-	0/2/5/7	-
1	CSX	B	196	1	-	0/2/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	450	1	15,15,16	0.99	1 (6%)	21,22,23	1.22	3 (14%)
2	PLP	A	450	1	15,15,16	1.21	3 (20%)	21,22,23	1.42	2 (9%)
3	KAP	B	451	-	11,12,12	0.63	0	11,14,14	1.93	3 (27%)
3	KAP	A	451	-	11,12,12	0.73	0	11,14,14	1.87	3 (27%)

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	450	1	-	0/6/6/8	0/1/1/1
2	PLP	A	450	1	-	0/6/6/8	0/1/1/1
3	KAP	B	451	-	-	6/10/12/12	-
3	KAP	A	451	-	-	5/10/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	PLP	C2-N1	2.60	1.38	1.33
2	B	450	PLP	C2-N1	2.29	1.37	1.33
2	A	450	PLP	C6-N1	2.11	1.38	1.34
2	A	450	PLP	C3-C2	-2.07	1.38	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	451	KAP	CD-CE-CZ	-4.18	106.81	114.50
3	A	451	KAP	CD-CE-CZ	-3.87	107.39	114.50
2	A	450	PLP	O4P-C5A-C5	3.83	116.53	109.36
3	A	451	KAP	CS-CH-CZ	2.92	113.89	109.67
3	B	451	KAP	CS-CH-CZ	2.64	113.48	109.67
2	B	450	PLP	O4P-C5A-C5	2.51	114.06	109.36
3	A	451	KAP	CB-CA-C	-2.48	108.03	114.51
3	B	451	KAP	CB-CA-C	-2.23	108.68	114.51
2	B	450	PLP	C6-C5-C4	2.06	119.79	118.10
2	A	450	PLP	C2A-C2-C3	-2.05	118.40	120.80
2	B	450	PLP	C5-C6-N1	-2.00	120.57	123.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	451	KAP	CA-CB-CG-CD
3	B	451	KAP	CS-CH-CZ-O
3	A	451	KAP	CE-CD-CG-CB
3	A	451	KAP	CA-CB-CG-CD
3	A	451	KAP	CS-CH-CZ-O
3	A	451	KAP	CS-CH-CZ-CE
3	B	451	KAP	CS-CH-CZ-CE

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Mol	Chain	Res	Type	Atoms
3	B	451	KAP	CD-CE-CZ-CH
3	B	451	KAP	CE-CD-CG-CB
3	A	451	KAP	C-CA-CB-CG
3	B	451	KAP	CD-CE-CZ-O

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	450	PLP	1	0
3	B	451	KAP	1	0
3	A	451	KAP	1	0

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 [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	447/448 (99%)	-0.01	9 (2%) 65 62	16, 27, 45, 76	4 (0%)
1	B	447/448 (99%)	-0.14	5 (1%) 78 76	12, 25, 42, 79	0
All	All	894/896 (99%)	-0.08	14 (1%) 70 67	12, 26, 45, 79	4 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	448	ASP	4.4
1	A	1	MET	3.6
1	A	195	GLN	3.5
1	A	192	CYS	3.4
1	B	188	ASP	3.0
1	B	1	MET	2.5
1	A	188	ASP	2.4
1	A	180	TYR	2.3
1	B	309	LEU	2.2
1	B	191	GLU	2.1
1	A	164	HIS	2.1
1	A	178	ILE	2.1
1	A	165	VAL	2.1
1	A	3	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSX	A	196	7/8	0.90	0.09	29,33,41,46	0
1	CSX	B	196	7/8	0.96	0.07	20,28,31,33	0

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	KAP	A	451	13/13	0.84	0.12	32,36,46,49	0
3	KAP	B	451	13/13	0.85	0.11	30,35,41,43	0
2	PLP	A	450	15/16	0.97	0.06	23,26,32,33	0
2	PLP	B	450	15/16	0.97	0.06	21,27,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.