



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:53 PM GMT

PDB ID : 1R43
Title : Crystal structure of beta-alanine synthase from *Saccharomyces kluyveri* (selenomethionine substituted protein)
Authors : Lundgren, S.; Gojkovic, Z.; Piskur, J.; Dobritsch, D.
Deposited on : 2003-10-03
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

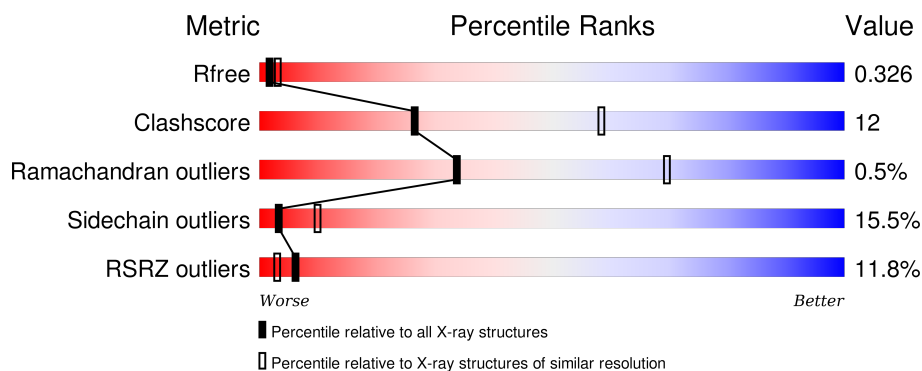
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	463	
1	B	463	

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
4	TRS	A	504	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6818 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 beta-alanine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	Se	0	0	0
			3379	2130	580	653	8	8			
1	B	432	Total	C	N	O	S	Se	0	0	0
			3337	2103	573	645	8	8			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
A	61	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
A	73	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
A	96	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
A	187	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
A	277	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
A	281	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
A	332	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
A	410	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
A	456	HIS	-	EXPRESSION TAG	UNP Q96W94
A	457	HIS	-	EXPRESSION TAG	UNP Q96W94
A	458	HIS	-	EXPRESSION TAG	UNP Q96W94
A	459	HIS	-	EXPRESSION TAG	UNP Q96W94
A	460	HIS	-	EXPRESSION TAG	UNP Q96W94
A	461	HIS	-	EXPRESSION TAG	UNP Q96W94
A	462	HIS	-	EXPRESSION TAG	UNP Q96W94
A	463	HIS	-	EXPRESSION TAG	UNP Q96W94
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
B	61	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
B	73	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
B	96	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
B	187	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
B	277	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
B	281	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
B	332	MSE	MET	MODIFIED RESIDUE	UNP Q96W94

Continued on next page...

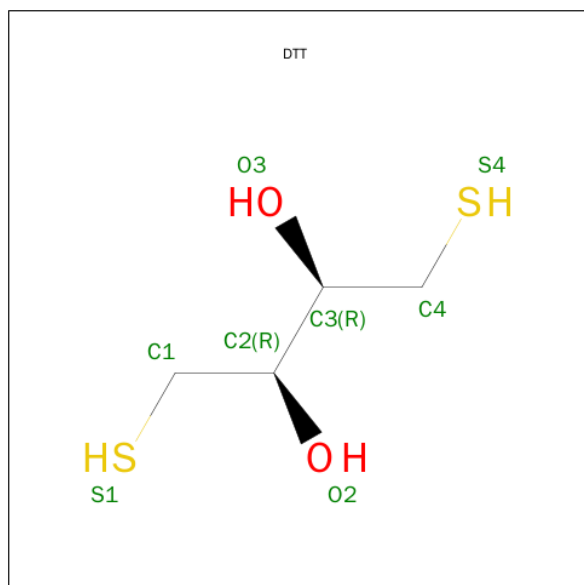
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	410	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
B	456	HIS	-	EXPRESSION TAG	UNP Q96W94
B	457	HIS	-	EXPRESSION TAG	UNP Q96W94
B	458	HIS	-	EXPRESSION TAG	UNP Q96W94
B	459	HIS	-	EXPRESSION TAG	UNP Q96W94
B	460	HIS	-	EXPRESSION TAG	UNP Q96W94
B	461	HIS	-	EXPRESSION TAG	UNP Q96W94
B	462	HIS	-	EXPRESSION TAG	UNP Q96W94
B	463	HIS	-	EXPRESSION TAG	UNP Q96W94

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

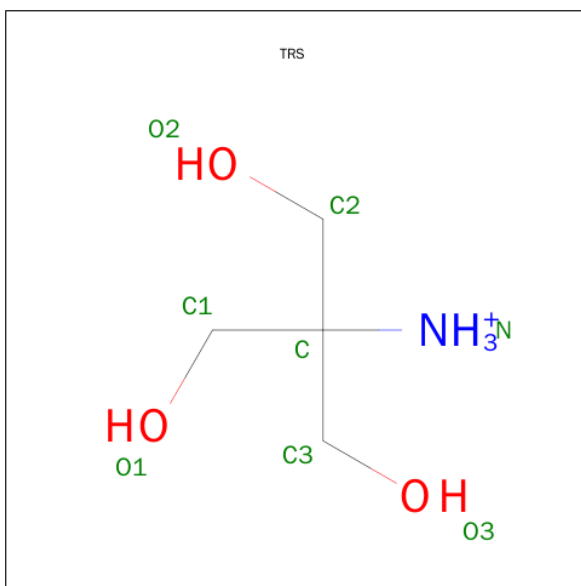
- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		

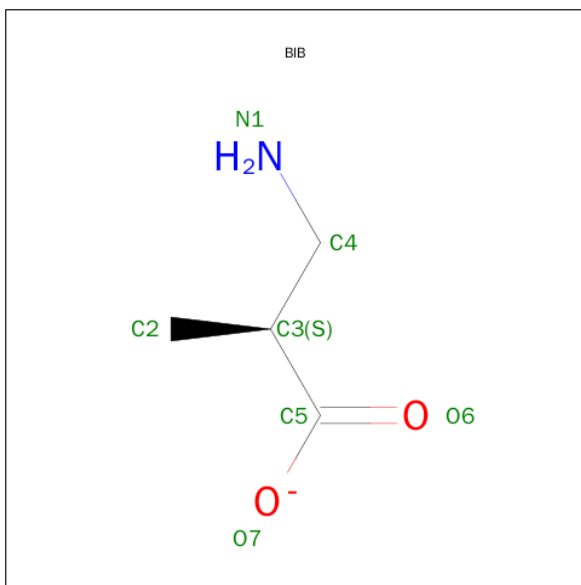
- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is BETA-AMINO ISOBUTYRATE (three-letter code: BIB) (formula: $C_4H_8NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	4	1	2		
5	B	1	Total	C	N	O	0	0
			7	4	1	2		

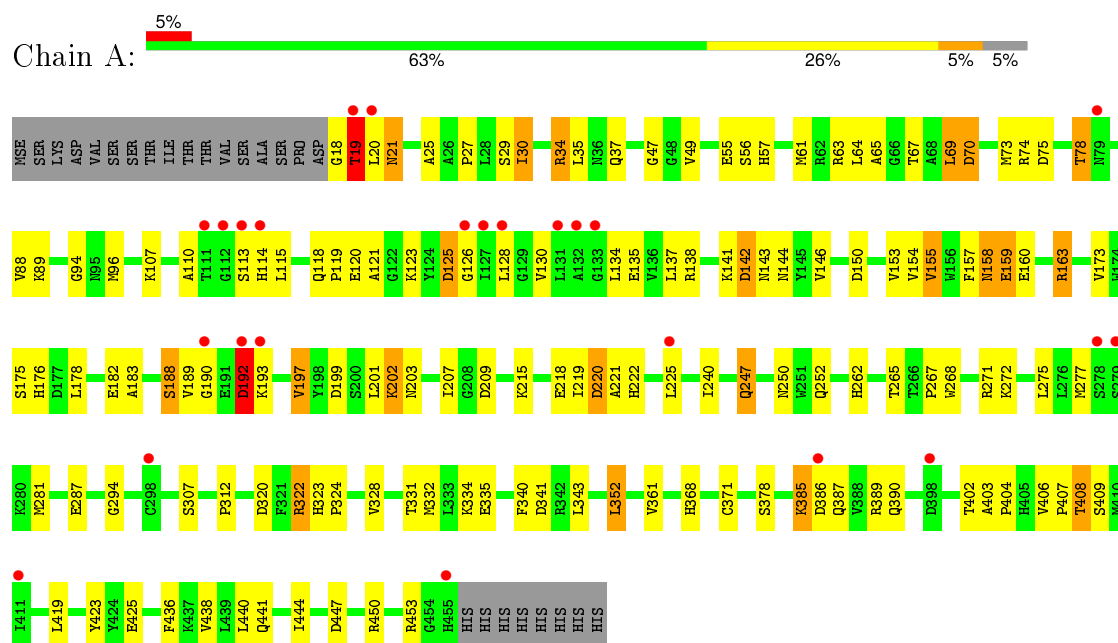
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total 54	O 54	0	0
6	B	14	Total 14	O 14	0	0

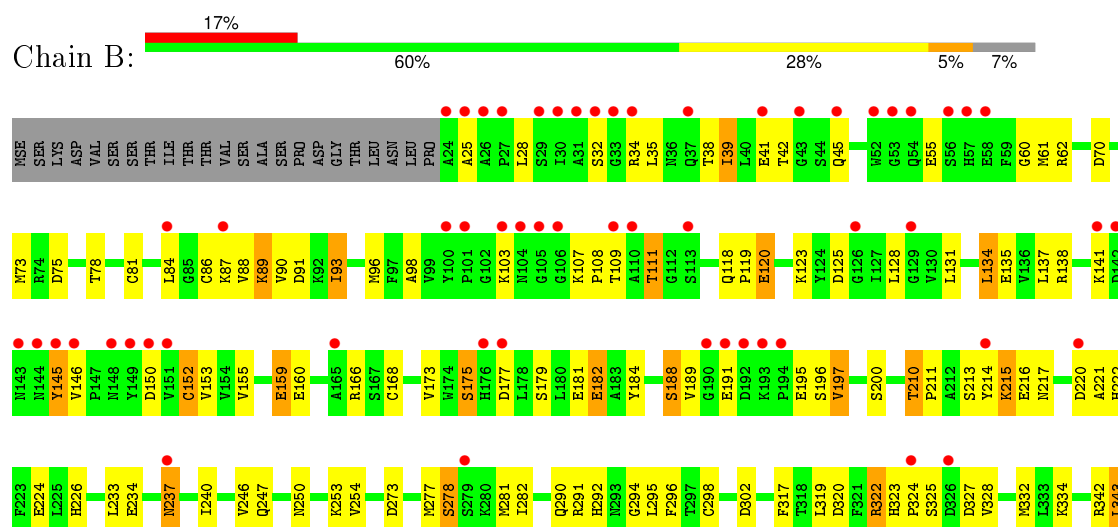
3 Residue-property plots [i](#)

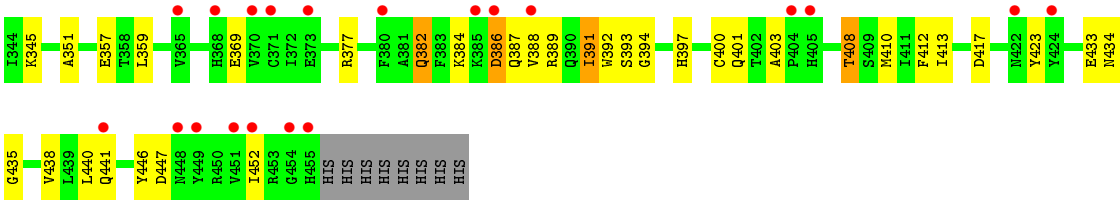
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: beta-alanine synthase



• Molecule 1: beta-alanine synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.43 Å 77.63 Å 110.57 Å 90.00° 95.63° 90.00°	Depositor
Resolution (Å)	29.75 – 2.80 28.73 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.75-2.80) 99.2 (28.73-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.211 , 0.274 0.286 , 0.326	Depositor DCC
R_{free} test set	1275 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 13.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25094 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6818	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, BIB, TRS, DTT

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	0.54	0/3449	0.79	9/4665 (0.2%)
1	B	0.43	0/3406	0.74	11/4605 (0.2%)
All	All	0.49	0/6855	0.76	20/9270 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CB-CG-OD2	7.15	124.73	118.30
1	B	320	ASP	CB-CG-OD2	6.36	124.03	118.30
1	A	220	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	192	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	386	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	341	ASP	CB-CG-OD2	5.86	123.58	118.30
1	B	177	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	386	ASP	CB-CG-OD2	5.64	123.37	118.30
1	B	220	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	273	ASP	CB-CG-OD2	5.63	123.36	118.30
1	B	447	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	417	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	70	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	142	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	150	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	327	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	70	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	302	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	447	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	75	ASP	CB-CG-OD2	5.02	122.82	118.30

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	3379	0	3263	87	0
1	B	3337	0	3219	80	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	8	0	9	0	0
4	A	8	0	12	0	0
5	A	7	0	8	0	0
5	B	7	0	8	0	0
6	A	54	0	0	2	0
6	B	14	0	0	1	0
All	All	6818	0	6519	162	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 12.

All (162) 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:35:LEU:HB2	1:A:135:GLU:HG3	1.54	0.88
1:A:371:CYS:HB3	1:A:409:SER:HB2	1.57	0.87
1:A:323:HIS:CD2	1:A:332:MSE:HE1	2.14	0.83
1:A:240:ILE:HG12	1:A:438:VAL:HG21	1.61	0.80
1:B:108:PRO:HB2	1:B:152:CYS:HB3	1.67	0.76
1:A:323:HIS:HD2	1:A:332:MSE:HE1	1.49	0.75
1:A:118:GLN:HG3	1:A:119:PRO:HD2	1.70	0.72
1:A:135:GLU:HG2	6:A:542:HOH:O	1.90	0.69
1:A:371:CYS:CB	1:A:409:SER:HB2	2.21	0.69
1:A:118:GLN:HG2	6:A:552:HOH:O	1.92	0.69
1:A:183:ALA:O	1:A:197:VAL:HG21	1.93	0.68
1:B:328:VAL:HG12	1:B:332:MSE:HE3	1.74	0.68
1:A:403:ALA:HA	1:A:408:THR:HG23	1.75	0.67
1:B:413:ILE:HD11	1:B:435:GLY:HA3	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:CYS:HB3	1:A:409:SER:CB	2.24	0.66
1:B:240:ILE:HG12	1:B:438:VAL:HG21	1.79	0.64
1:A:323:HIS:CD2	1:A:332:MSE:CE	2.80	0.64
1:A:115:LEU:HD21	1:A:130:VAL:HG11	1.78	0.64
1:A:201:LEU:HB3	1:A:207:ILE:HG13	1.79	0.64
1:B:277:MSE:CE	1:B:343:LEU:HB3	2.28	0.63
1:A:328:VAL:HG12	1:A:332:MSE:HE3	1.80	0.63
1:B:403:ALA:HA	1:B:408:THR:CG2	2.29	0.63
1:B:277:MSE:HE1	1:B:343:LEU:HB3	1.79	0.62
1:B:254:VAL:HG11	1:B:281:MSE:HE1	1.81	0.62
1:B:118:GLN:HG3	1:B:119:PRO:HD2	1.80	0.62
1:A:67:THR:HG23	1:A:69:LEU:H	1.65	0.61
1:A:21:ASN:HD22	1:A:21:ASN:N	1.98	0.61
1:B:108:PRO:CB	1:B:152:CYS:HB3	2.30	0.61
1:A:402:THR:OG1	1:A:408:THR:HG21	2.01	0.61
1:A:120:GLU:HA	1:A:423:TYR:CE2	2.35	0.61
1:A:74:ARG:HH11	1:A:96:MSE:HE2	1.66	0.60
1:B:96:MSE:HB2	1:B:155:VAL:CG1	2.32	0.59
1:A:21:ASN:HD22	1:A:21:ASN:H	1.50	0.59
1:B:28:LEU:HD21	1:B:145:TYR:CE1	2.38	0.59
1:A:368:HIS:CG	1:A:407:PRO:HB3	2.38	0.58
1:A:219:ILE:HG13	1:A:406:VAL:HG11	1.86	0.58
1:B:222:HIS:HB3	1:B:408:THR:HB	1.84	0.58
1:B:111:THR:O	1:B:153:VAL:HA	2.03	0.58
1:A:74:ARG:NH1	1:A:96:MSE:HE2	2.19	0.58
1:A:294:GLY:HA3	1:A:332:MSE:HE1	1.84	0.58
1:B:98:ALA:O	1:B:152:CYS:HA	2.05	0.57
1:B:42:THR:HB	1:B:73:MSE:SE	2.55	0.57
1:A:115:LEU:HD12	1:A:155:VAL:HG21	1.87	0.56
1:A:74:ARG:NH1	1:A:94:GLY:O	2.37	0.56
1:B:134:LEU:HD22	1:B:138:ARG:HE	1.71	0.56
1:B:294:GLY:HA3	1:B:332:MSE:HE1	1.86	0.56
1:A:74:ARG:NH1	1:A:96:MSE:CE	2.68	0.56
1:B:160:GLU:OE1	1:B:160:GLU:HA	2.06	0.56
1:B:91:ASP:HA	1:B:210:THR:O	2.06	0.55
1:B:292:HIS:HB2	1:B:332:MSE:HE2	1.87	0.55
1:A:176:HIS:CE1	1:A:215:LYS:HD2	2.42	0.55
1:A:406:VAL:HG23	1:A:408:THR:HG22	1.89	0.54
1:B:125:ASP:OD1	1:B:226:HIS:CE1	2.60	0.54
1:B:188:SER:HB2	1:B:195:GLU:H	1.72	0.54
1:A:183:ALA:O	1:A:197:VAL:CG2	2.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLN:HG3	1:B:119:PRO:CD	2.39	0.52
1:A:368:HIS:CD2	1:A:407:PRO:HB3	2.45	0.52
1:B:323:HIS:CD2	1:B:332:MSE:HE1	2.46	0.51
1:B:233:LEU:HD11	1:B:412:PHE:HB3	1.92	0.51
1:A:199:ASP:O	1:A:203:ASN:HB2	2.09	0.51
1:A:135:GLU:OE1	1:A:138:ARG:HD3	2.10	0.51
1:A:25:ALA:O	1:A:27:PRO:HD3	2.11	0.51
1:B:96:MSE:HB2	1:B:155:VAL:HG12	1.92	0.50
1:B:135:GLU:HA	1:B:138:ARG:HB2	1.92	0.50
1:B:35:LEU:HB2	1:B:135:GLU:HG3	1.92	0.50
1:A:96:MSE:HB2	1:A:155:VAL:HG13	1.92	0.50
1:B:213:SER:HB3	1:B:216:GLU:HG3	1.94	0.50
1:A:189:VAL:HG23	1:A:190:GLY:N	2.27	0.50
1:B:397:HIS:O	1:B:400:CYS:HB2	2.11	0.50
1:A:277:MSE:HE3	1:A:352:LEU:HG	1.93	0.50
1:A:267:PRO:HA	1:B:295:LEU:HD21	1.95	0.49
1:A:63:ARG:CZ	1:A:73:MSE:HG2	2.41	0.49
1:A:78:THR:HB	1:A:88:VAL:HG21	1.94	0.49
1:B:397:HIS:ND1	6:B:1512:HOH:O	2.29	0.49
1:A:143:ASN:O	1:A:144:ASN:HB2	2.13	0.49
1:B:246:VAL:HG22	1:B:393:SER:HB3	1.94	0.49
1:A:110:ALA:HB3	1:A:221:ALA:O	2.12	0.48
1:A:275:LEU:HD23	1:B:298:CYS:O	2.13	0.48
1:B:60:GLY:O	1:B:61:MSE:HE2	2.13	0.48
1:A:247:GLN:HE21	1:A:324:PRO:HD3	1.79	0.48
1:B:224:GLU:HB3	1:B:410:MSE:HG2	1.96	0.48
1:A:57:HIS:O	1:A:123:LYS:NZ	2.41	0.48
1:A:159:GLU:OE2	1:A:160:GLU:HA	2.14	0.48
1:A:378:SER:OG	1:A:441:GLN:HB2	2.13	0.47
1:A:320:ASP:OD1	1:A:322:ARG:HD2	2.14	0.47
1:A:137:LEU:HD11	1:A:153:VAL:HG23	1.95	0.47
1:A:262:HIS:HE1	1:B:322:ARG:NH2	2.12	0.47
1:B:120:GLU:HG3	1:B:423:TYR:CZ	2.49	0.47
1:B:28:LEU:HD21	1:B:145:TYR:CD1	2.50	0.47
1:B:323:HIS:HD2	1:B:332:MSE:HE1	1.80	0.47
1:B:78:THR:HG22	1:B:88:VAL:HG11	1.96	0.47
1:B:253:LYS:HB2	1:B:359:LEU:HD11	1.97	0.47
1:B:184:TYR:HA	1:B:197:VAL:HG22	1.97	0.47
1:A:128:LEU:HD21	1:A:225:LEU:HG	1.97	0.46
1:B:78:THR:CG2	1:B:96:MSE:HE3	2.45	0.46
1:B:120:GLU:HA	1:B:423:TYR:CE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ALA:HA	1:A:408:THR:CG2	2.43	0.46
1:B:93:ILE:CD1	1:B:173:VAL:HB	2.46	0.46
1:B:296:PHE:HE1	1:B:319:LEU:CD2	2.29	0.46
1:A:403:ALA:N	1:A:404:PRO:CD	2.79	0.45
1:B:78:THR:HG23	1:B:96:MSE:HE3	1.97	0.45
1:A:74:ARG:HH22	1:A:157:PHE:HA	1.81	0.45
1:A:163:ARG:O	1:A:188:SER:HA	2.15	0.45
1:B:382:GLN:HE22	1:B:441:GLN:HG3	1.82	0.45
1:A:202:LYS:HB2	1:A:207:ILE:HD12	1.98	0.45
1:B:38:THR:HG21	1:B:138:ARG:HH22	1.81	0.45
1:B:159:GLU:HA	1:B:168:CYS:HA	1.98	0.45
1:A:175:SER:O	1:A:176:HIS:HB2	2.17	0.45
1:B:93:ILE:HD13	1:B:173:VAL:HB	1.99	0.44
1:B:281:MSE:HE2	1:B:317:PHE:CZ	2.52	0.44
1:B:434:ASN:O	1:B:438:VAL:HG23	2.18	0.44
1:A:64:LEU:O	1:A:67:THR:HG22	2.18	0.44
1:A:47:GLY:HA3	1:A:61:MSE:CE	2.48	0.44
1:A:192:ASP:OD1	1:A:192:ASP:N	2.50	0.44
1:A:30:ILE:HG12	1:A:436:PHE:HE2	1.83	0.43
1:A:385:LYS:HA	1:A:385:LYS:HD3	1.80	0.43
1:B:90:VAL:O	1:B:210:THR:HG23	2.18	0.43
1:A:281:MSE:HE2	1:A:340:PHE:HB3	1.99	0.43
1:B:96:MSE:HB2	1:B:155:VAL:HG13	2.00	0.43
1:B:93:ILE:HD11	1:B:173:VAL:HG11	2.00	0.43
1:A:268:TRP:NE1	1:B:294:GLY:O	2.51	0.43
1:B:78:THR:HG23	1:B:96:MSE:CE	2.48	0.43
1:B:221:ALA:HB2	1:B:446:TYR:CZ	2.53	0.43
1:A:123:LYS:HB2	1:A:123:LYS:HE2	1.78	0.43
1:B:175:SER:OG	1:B:401:GLN:HB3	2.18	0.43
1:A:173:VAL:HG22	1:A:178:LEU:HB3	2.00	0.43
1:B:111:THR:HG23	1:B:153:VAL:HG22	2.01	0.43
1:B:39:ILE:HG13	1:B:131:LEU:HD12	2.01	0.43
1:A:275:LEU:CB	1:A:312:PRO:HG2	2.49	0.43
1:B:214:TYR:CE2	1:B:215:LYS:HE3	2.54	0.43
1:B:84:LEU:HA	1:B:141:LYS:HE2	2.00	0.42
1:A:65:ALA:HB1	1:A:158:ASN:HB2	2.01	0.42
1:A:222:HIS:HB3	1:A:408:THR:HB	2.02	0.42
1:A:35:LEU:CD2	1:A:436:PHE:HB2	2.49	0.42
1:A:125:ASP:HB2	1:A:425:GLU:OE2	2.19	0.42
1:B:89:LYS:HB3	1:B:210:THR:HG21	2.02	0.42
1:B:84:LEU:HD13	1:B:137:LEU:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:CYS:HB3	1:B:86:CYS:SG	2.59	0.42
1:A:265:THR:HA	1:B:394:GLY:HA3	2.01	0.42
1:B:184:TYR:O	1:B:196:SER:HB2	2.20	0.42
1:B:345:LYS:HD3	1:B:351:ALA:HB2	2.02	0.42
1:B:179:SER:OG	1:B:182:GLU:HB2	2.20	0.42
1:A:70:ASP:O	1:A:74:ARG:HG3	2.20	0.42
1:A:18:GLY:O	1:A:19:THR:C	2.58	0.42
1:B:119:PRO:O	1:B:120:GLU:HB2	2.19	0.41
1:A:74:ARG:O	1:A:75:ASP:C	2.59	0.41
1:B:391:ILE:HG22	1:B:392:TRP:N	2.35	0.41
1:A:114:HIS:CE1	1:A:126:GLY:HA3	2.56	0.41
1:A:118:GLN:O	1:A:121:ALA:HB2	2.21	0.41
1:A:331:THR:O	1:A:335:GLU:HG3	2.21	0.41
1:B:323:HIS:CG	1:B:324:PRO:HD2	2.56	0.41
1:A:74:ARG:O	1:A:78:THR:HG23	2.21	0.41
1:B:38:THR:HG22	1:B:131:LEU:HD13	2.02	0.41
1:B:210:THR:HA	1:B:211:PRO:HD3	1.96	0.41
1:A:272:LYS:HB3	1:A:352:LEU:HD22	2.03	0.41
1:B:296:PHE:HE1	1:B:319:LEU:HD22	1.84	0.41
1:A:34:ARG:HA	1:A:37:GLN:HB3	2.02	0.41
1:A:440:LEU:O	1:A:444:ILE:HG13	2.21	0.41
1:A:21:ASN:N	1:A:21:ASN:ND2	2.68	0.40
1:A:176:HIS:HE1	1:A:215:LYS:HD2	1.85	0.40
1:A:61:MSE:HG3	1:A:123:LYS:HA	2.04	0.40
1:B:278:SER:O	1:B:282:ILE:HG13	2.21	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	436/463 (94%)	404 (93%)	30 (7%)	2 (0%)	34 69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	430/463 (93%)	395 (92%)	33 (8%)	2 (0%)	34	69
All	All	866/926 (94%)	799 (92%)	63 (7%)	4 (0%)	34	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	B	237	ASN
1	B	25	ALA
1	A	158	ASN

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	360/375 (96%)	310 (86%)	50 (14%)	4	13
1	B	355/375 (95%)	294 (83%)	61 (17%)	2	7
All	All	715/750 (95%)	604 (84%)	111 (16%)	3	10

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	20	LEU
1	A	21	ASN
1	A	29	SER
1	A	30	ILE
1	A	34	ARG
1	A	49	VAL
1	A	55	GLU
1	A	56	SER
1	A	69	LEU
1	A	78	THR
1	A	89	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	107	LYS
1	A	113	SER
1	A	134	LEU
1	A	141	LYS
1	A	142	ASP
1	A	146	VAL
1	A	154	VAL
1	A	155	VAL
1	A	159	GLU
1	A	163	ARG
1	A	182	GLU
1	A	188	SER
1	A	192	ASP
1	A	193	LYS
1	A	197	VAL
1	A	202	LYS
1	A	209	ASP
1	A	218	GLU
1	A	220	ASP
1	A	247	GLN
1	A	250	ASN
1	A	252	GLN
1	A	271	ARG
1	A	287	GLU
1	A	307	SER
1	A	322	ARG
1	A	334	LYS
1	A	343	LEU
1	A	352	LEU
1	A	361	VAL
1	A	385	LYS
1	A	387	GLN
1	A	389	ARG
1	A	390	GLN
1	A	408	THR
1	A	419	LEU
1	A	450	ARG
1	A	453	ARG
1	B	32	SER
1	B	34	ARG
1	B	39	ILE
1	B	41	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	45	GLN
1	B	55	GLU
1	B	62	ARG
1	B	87	LYS
1	B	89	LYS
1	B	93	ILE
1	B	103	LYS
1	B	107	LYS
1	B	109	THR
1	B	111	THR
1	B	120	GLU
1	B	123	LYS
1	B	128	LEU
1	B	134	LEU
1	B	145	TYR
1	B	146	VAL
1	B	150	ASP
1	B	152	CYS
1	B	159	GLU
1	B	166	ARG
1	B	175	SER
1	B	181	GLU
1	B	182	GLU
1	B	188	SER
1	B	189	VAL
1	B	191	GLU
1	B	197	VAL
1	B	200	SER
1	B	210	THR
1	B	215	LYS
1	B	217	ASN
1	B	234	GLU
1	B	237	ASN
1	B	247	GLN
1	B	250	ASN
1	B	278	SER
1	B	290	GLN
1	B	291	ARG
1	B	322	ARG
1	B	325	SER
1	B	334	LYS
1	B	342	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	343	LEU
1	B	357	GLU
1	B	369	GLU
1	B	377	ARG
1	B	382	GLN
1	B	384	LYS
1	B	386	ASP
1	B	387	GLN
1	B	388	VAL
1	B	389	ARG
1	B	391	ILE
1	B	408	THR
1	B	433	GLU
1	B	440	LEU
1	B	452	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	250	ASN
1	B	57	HIS
1	B	250	ASN
1	B	382	GLN
1	B	441	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	DTT	A	503	1	7,7,7	0.56	0	4,8,8	1.62	0
4	TRS	A	504	-	7,7,7	1.00	1 (14%)	9,9,9	0.84	1 (11%)
5	BIB	A	505	-	3,6,6	0.43	0	1,7,7	0.47	0
5	BIB	B	1505	-	3,6,6	0.51	0	1,7,7	0.33	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	DTT	A	503	1	-	0/8/8/8	0/0/0/0
4	TRS	A	504	-	-	0/9/9/9	0/0/0/0
5	BIB	A	505	-	-	0/1/6/6	0/0/0/0
5	BIB	B	1505	-	-	0/1/6/6	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	TRS	C-N	-2.55	1.46	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	TRS	O2-C2-C	-2.12	106.89	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	430/463 (92%)	0.44	24 (5%) 28 18	14, 20, 24, 31	0
1	B	424/463 (91%)	1.06	77 (18%) 2 1	16, 20, 22, 29	0
All	All	854/926 (92%)	0.75	101 (11%) 6 3	14, 20, 23, 31	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	455	HIS	7.2
1	B	53	GLY	5.9
1	B	54	GLN	5.2
1	B	104	ASN	5.0
1	B	25	ALA	4.5
1	B	43	GLY	4.5
1	B	33	GLY	4.5
1	B	454	GLY	4.3
1	B	452	ILE	4.2
1	B	32	SER	4.1
1	B	145	TYR	4.1
1	B	37	GLN	4.1
1	B	105	GLY	3.9
1	B	106	GLY	3.8
1	B	451	VAL	3.8
1	B	214	TYR	3.7
1	B	103	LYS	3.7
1	B	190	GLY	3.6
1	B	56	SER	3.6
1	B	149	TYR	3.6
1	B	148	ASN	3.6
1	B	424	TYR	3.5
1	B	368	HIS	3.5
1	B	41	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	113	SER	3.4
1	B	380	PHE	3.4
1	B	101	PRO	3.3
1	B	27	PRO	3.3
1	B	386	ASP	3.3
1	A	190	GLY	3.2
1	B	143	ASN	3.2
1	B	324	PRO	3.2
1	B	144	ASN	3.2
1	B	326	ASP	3.2
1	B	58	GLU	3.2
1	B	57	HIS	3.2
1	B	31	ALA	3.1
1	A	19	THR	3.0
1	A	278	SER	3.0
1	B	45	GLN	3.0
1	B	388	VAL	3.0
1	B	84	LEU	3.0
1	B	30	ILE	3.0
1	A	112	GLY	2.9
1	B	176	HIS	2.9
1	B	449	TYR	2.9
1	B	192	ASP	2.8
1	A	192	ASP	2.8
1	B	113	SER	2.8
1	B	24	ALA	2.8
1	B	100	TYR	2.7
1	B	193	LYS	2.7
1	A	455	HIS	2.7
1	B	142	ASP	2.6
1	B	150	ASP	2.6
1	B	373	GLU	2.5
1	B	146	VAL	2.5
1	B	279	SER	2.5
1	A	114	HIS	2.5
1	B	441	GLN	2.5
1	A	193	LYS	2.5
1	A	20	LEU	2.5
1	B	52	TRP	2.4
1	A	225	LEU	2.4
1	A	126	GLY	2.4
1	B	385	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	151	VAL	2.4
1	A	279	SER	2.4
1	B	126	GLY	2.4
1	B	220	ASP	2.4
1	B	29	SER	2.4
1	B	371	CYS	2.4
1	B	87	LYS	2.3
1	B	177	ASP	2.3
1	B	370	VAL	2.3
1	B	165	ALA	2.3
1	B	109	THR	2.3
1	B	34	ARG	2.3
1	B	365	VAL	2.3
1	B	404	PRO	2.3
1	A	111	THR	2.2
1	A	131	LEU	2.2
1	B	194	PRO	2.2
1	A	79	ASN	2.2
1	B	129	GLY	2.2
1	B	26	ALA	2.2
1	B	110	ALA	2.2
1	A	132	ALA	2.2
1	B	237	ASN	2.2
1	B	422	ASN	2.1
1	B	448	ASN	2.1
1	B	141	LYS	2.1
1	A	128	LEU	2.1
1	B	405	HIS	2.1
1	A	411	ILE	2.1
1	A	386	ASP	2.1
1	B	191	GLU	2.1
1	A	133	GLY	2.0
1	A	298	CYS	2.0
1	A	398	ASP	2.0
1	A	127	ILE	2.0

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 [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	TRS	A	504	8/8	0.71	0.38	12.13	19,20,20,20	0
3	DTT	A	503	8/8	0.75	0.29	0.83	30,31,31,33	0
5	BIB	A	505	7/7	0.82	0.26	0.31	15,18,18,18	0
2	ZN	A	501	1/1	0.98	0.16	-1.28	28,28,28,28	0
5	BIB	B	1505	7/7	0.89	0.17	-1.33	19,19,20,20	0
2	ZN	A	500	1/1	0.97	0.20	-1.89	21,21,21,21	0
2	ZN	B	500	1/1	0.96	0.11	-2.03	20,20,20,20	0
2	ZN	B	501	1/1	0.96	0.05	-4.20	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.