



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:58 PM UTC

PDB ID : 1R43 / pdb_00001r43
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

<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

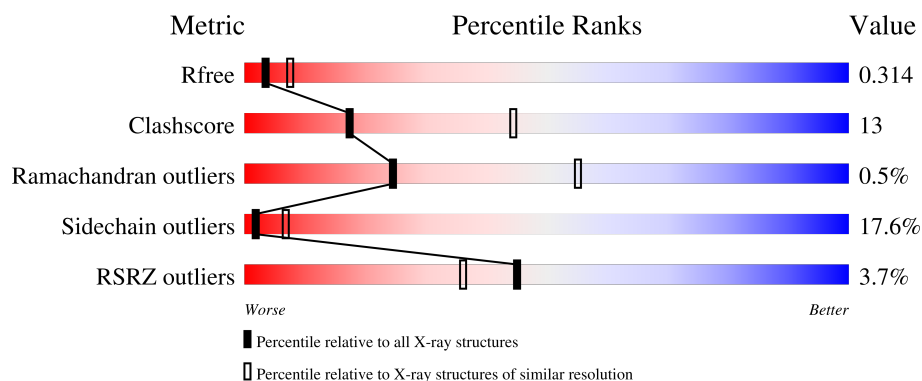
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	463	2% 62% 28% 5% 5%
1	B	463	5% 61% 27% 5% 7%

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

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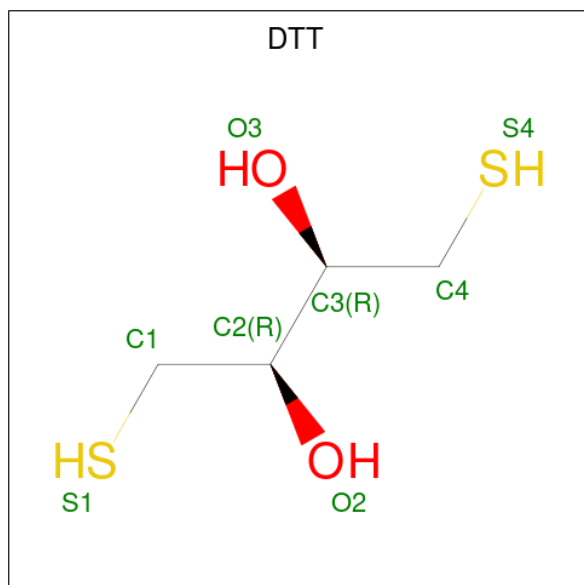
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Chain	Residue	Modelled	Actual	Comment	Reference
B	410	MSE	MET	modified residue	UNP Q96W94
B	456	HIS	-	expression tag	UNP Q96W94
B	457	HIS	-	expression tag	UNP Q96W94
B	458	HIS	-	expression tag	UNP Q96W94
B	459	HIS	-	expression tag	UNP Q96W94
B	460	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 (CCD ID: ZN) (formula: Zn).

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

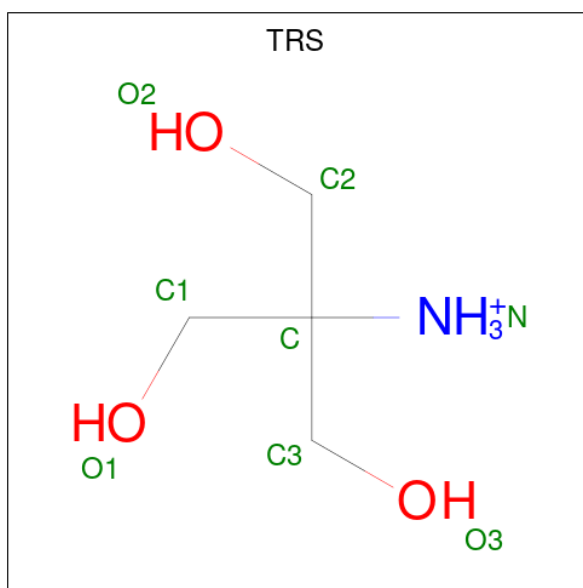
- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C₄H₁₀O₂S₂).



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

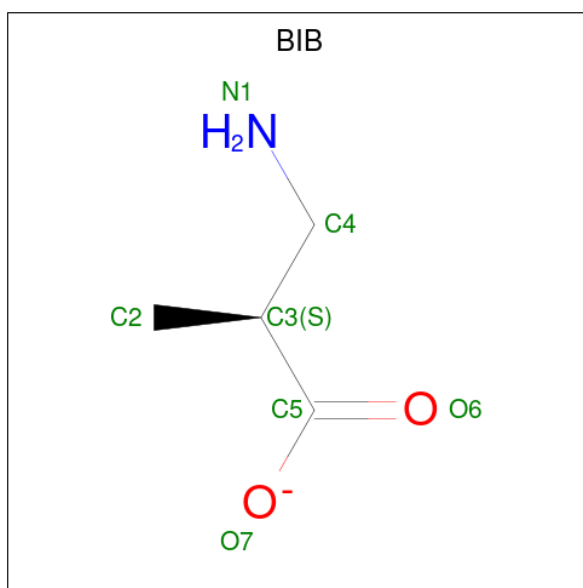
- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS)

(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 (CCD ID: 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		

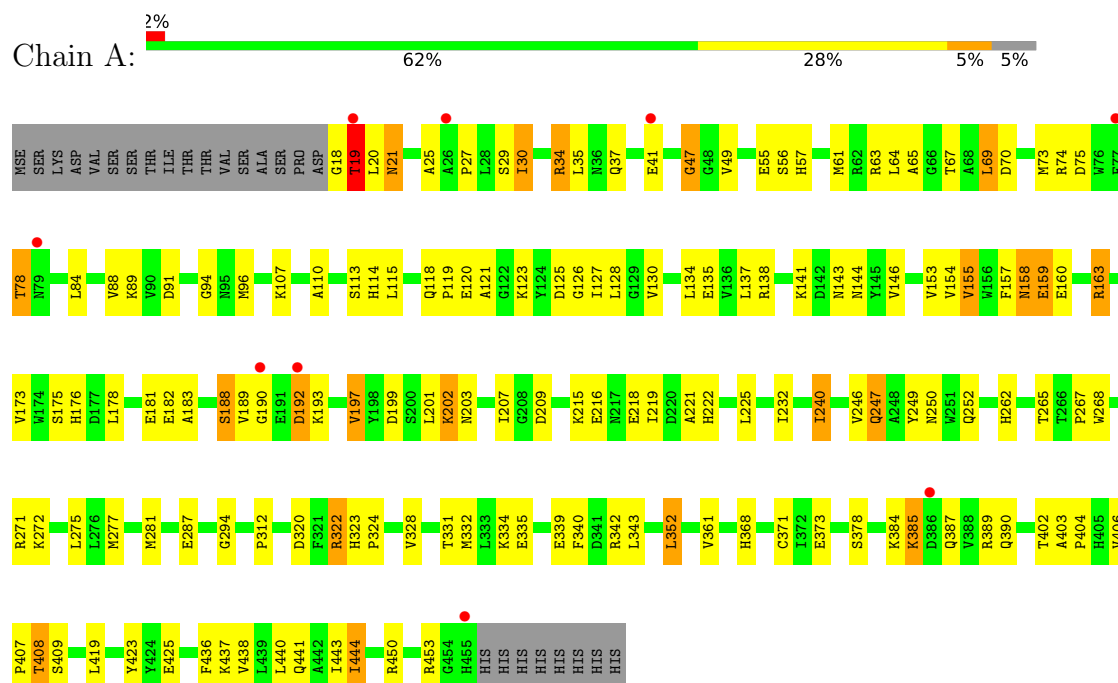
- Molecule 6 is water.

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

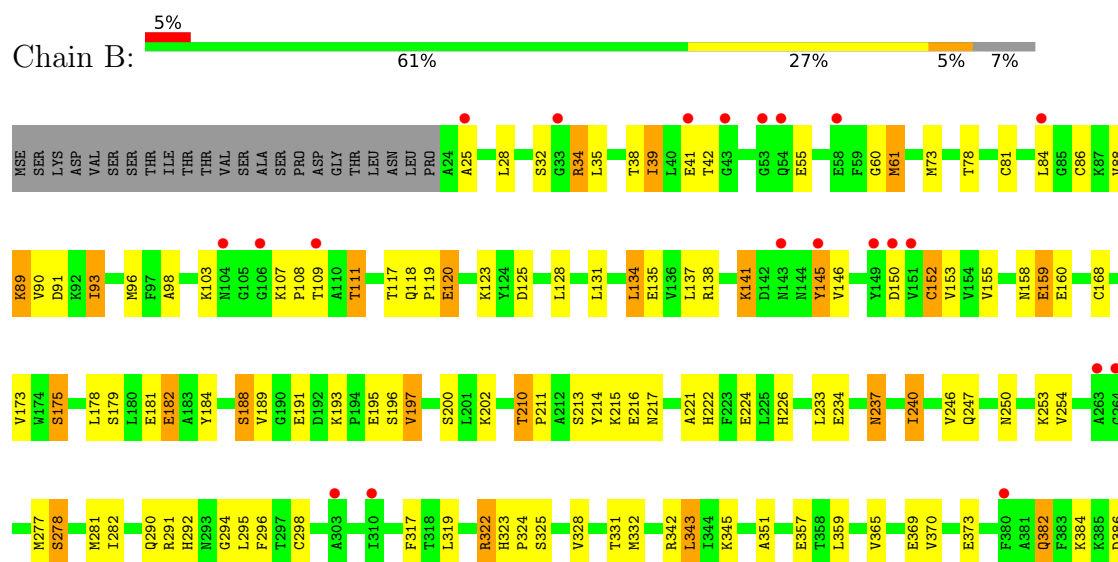
3 Residue-property plots

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: beta-alanine synthase



• Molecule 1: beta-alanine synthase



Q387	V388	R389	Q390	I391	W392	S393	G394		H397		C400	Q401	T402	A403		V406	F407	T408	S409	N410	T411	F412	I413		Y423		I432	E433	N434	G435		V438	L439	L440	Q441		Y446		V451	I452	R453	G454	H455		HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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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	60.43Å 77.63Å 110.57Å 90.00° 95.63° 90.00°	Depositor
Resolution (Å)	29.75 – 2.80 29.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.75-2.80) 99.1 (29.75-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.211 , 0.274 0.285 , 0.314	Depositor DCC
R_{free} test set	1275 reflections (5.08%)	wwPDB-VP
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 , 10.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: BIB, DTT, TRS, ZN

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	0.69	0/3449	0.96	2/4665 (0.0%)
1	B	0.55	0/3406	0.93	3/4605 (0.1%)
All	All	0.63	0/6855	0.95	5/9270 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ILE	N-CA-C	6.61	117.30	110.36
1	A	47	GLY	N-CA-C	6.40	121.78	113.27
1	B	34	ARG	N-CA-C	6.08	117.71	111.14
1	B	158	ASN	N-CA-C	5.28	118.61	111.17
1	B	61	MSE	N-CA-C	5.07	117.17	108.90

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	90	0
1	B	3337	0	3219	81	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	166	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 13.

All (166) 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:118:GLN:HG2	6:A:552:HOH:O	1.92	0.69
1:A:371:CYS:CB	1:A:409:SER:HB2	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:PRO:CB	1:B:152:CYS:HB3	2.30	0.61
1:A:120:GLU:HA	1:A:423:TYR:CE2	2.35	0.61
1:A:402:THR:OG1	1:A:408:THR:HG21	2.01	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:111:THR:O	1:B:153:VAL:HA	2.03	0.58
1:B:222:HIS:HB3	1:B:408:THR:HB	1.84	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:A:74:ARG:NH1	1:A:96:MSE:CE	2.68	0.56
1:B:294:GLY:HA3	1:B:332:MSE:HE1	1.86	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
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:A:199:ASP:O	1:A:203:ASN:HB2	2.09	0.51
1:B:233:LEU:HD11	1:B:412:PHE:HB3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:247:GLN:HE21	1:A:324:PRO:HD3	1.79	0.48
1:B:60:GLY:O	1:B:61:MSE:HE2	2.13	0.48
1:A:57:HIS:O	1:A:123:LYS:NZ	2.41	0.48
1:B:224:GLU:HB3	1:B:410:MSE:HG2	1.96	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:28:LEU:HD21	1:B:145:TYR:CD1	2.50	0.47
1:B:120:GLU:HG3	1:B:423:TYR:CZ	2.49	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:184:TYR:HA	1:B:197:VAL:HG22	1.97	0.47
1:B:253:LYS:HB2	1:B:359:LEU:HD11	1.97	0.47
1:A:18:GLY:O	1:A:19:THR:C	2.58	0.46
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:A:74:ARG:O	1:A:75:ASP:C	2.59	0.46
1:B:120:GLU:HA	1:B:423:TYR:CE2	2.50	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:47:GLY:HA3	1:A:61:MSE:CE	2.48	0.44
1:A:64:LEU:O	1:A:67:THR:HG22	2.18	0.44
1:A:384:LYS:O	1:A:385:LYS:C	2.60	0.44
1:B:434:ASN:O	1:B:438:VAL:HG23	2.18	0.44
1:A:192:ASP:N	1:A:192:ASP:OD1	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:A:281:MSE:HE2	1:A:340:PHE:HB3	1.99	0.43
1:B:90:VAL:O	1:B:210:THR:HG23	2.18	0.43
1:B:117:THR:C	1:B:160:GLU:HG3	2.43	0.43
1:B:93:ILE:HD11	1:B:173:VAL:HG11	2.00	0.43
1:B:96:MSE:HB2	1:B:155:VAL:HG13	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:HE2	1:A:123:LYS:HB2	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:A:275:LEU:CB	1:A:312:PRO:HG2	2.49	0.43
1:B:39:ILE:HG13	1:B:131:LEU:HD12	2.01	0.43
1:B:214:TYR:CE2	1:B:215:LYS:HE3	2.54	0.43
1:A:65:ALA:HB1	1:A:158:ASN:HB2	2.01	0.42
1:B:84:LEU:HA	1:B:141:LYS:HE2	2.00	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:81:CYS:HB3	1:B:86:CYS:SG	2.59	0.42
1:B:84:LEU:HD13	1:B:137:LEU:HB2	2.02	0.42
1:B:89:LYS:HB3	1:B:210:THR:HG21	2.02	0.42
1:A:265:THR:HA	1:B:394:GLY:HA3	2.01	0.42
1:B:179:SER:OG	1:B:182:GLU:HB2	2.20	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:A:70:ASP:O	1:A:74:ARG:HG3	2.20	0.42
1:A:249:TYR:CD1	1:A:249:TYR:C	2.97	0.42
1:B:119:PRO:O	1:B:120:GLU:HB2	2.19	0.41
1:A:114:HIS:CE1	1:A:126:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ILE:HG22	1:B:392:TRP:N	2.35	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:A:91:ASP:OD1	1:A:91:ASP:C	2.64	0.41
1:B:323:HIS:CG	1:B:324:PRO:HD2	2.56	0.41
1:A:34:ARG:HA	1:A:37:GLN:HB3	2.02	0.41
1:A:74:ARG:O	1:A:78:THR:HG23	2.21	0.41
1:A:272:LYS:HB3	1:A:352:LEU:HD22	2.03	0.41
1:A:440:LEU:O	1:A:444:ILE:HG13	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:B:296:PHE:HE1	1:B:319:LEU:HD22	1.84	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%)	24	55
1	B	430/463 (93%)	395 (92%)	33 (8%)	2 (0%)	24	55
All	All	866/926 (94%)	799 (92%)	63 (7%)	4 (0%)	24	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	B	237	ASN

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Mol	Chain	Res	Type
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%)	300 (83%)	60 (17%)	2	8
1	B	355/375 (95%)	289 (81%)	66 (19%)	1	5
All	All	715/750 (95%)	589 (82%)	126 (18%)	2	7

All (126) 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	41	GLU
1	A	49	VAL
1	A	55	GLU
1	A	56	SER
1	A	69	LEU
1	A	78	THR
1	A	84	LEU
1	A	89	LYS
1	A	107	LYS
1	A	113	SER
1	A	127	ILE
1	A	134	LEU
1	A	141	LYS
1	A	146	VAL
1	A	154	VAL

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Mol	Chain	Res	Type
1	A	155	VAL
1	A	159	GLU
1	A	163	ARG
1	A	181	GLU
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	216	GLU
1	A	218	GLU
1	A	240	ILE
1	A	246	VAL
1	A	247	GLN
1	A	250	ASN
1	A	252	GLN
1	A	271	ARG
1	A	287	GLU
1	A	322	ARG
1	A	334	LYS
1	A	339	GLU
1	A	342	ARG
1	A	343	LEU
1	A	352	LEU
1	A	361	VAL
1	A	373	GLU
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	437	LYS
1	A	443	ILE
1	A	444	ILE
1	A	450	ARG
1	A	453	ARG
1	B	32	SER
1	B	34	ARG
1	B	39	ILE

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Mol	Chain	Res	Type
1	B	41	GLU
1	B	55	GLU
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	141	LYS
1	B	145	TYR
1	B	146	VAL
1	B	150	ASP
1	B	152	CYS
1	B	159	GLU
1	B	175	SER
1	B	178	LEU
1	B	181	GLU
1	B	182	GLU
1	B	188	SER
1	B	189	VAL
1	B	191	GLU
1	B	193	LYS
1	B	197	VAL
1	B	200	SER
1	B	202	LYS
1	B	210	THR
1	B	217	ASN
1	B	234	GLU
1	B	237	ASN
1	B	240	ILE
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	331	THR

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Mol	Chain	Res	Type
1	B	342	ARG
1	B	343	LEU
1	B	357	GLU
1	B	365	VAL
1	B	369	GLU
1	B	370	VAL
1	B	373	GLU
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	406	VAL
1	B	408	THR
1	B	432	ILE
1	B	433	GLU
1	B	440	LEU
1	B	451	VAL
1	B	452	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	57	HIS
1	A	247	GLN
1	A	250	ASN
1	A	293	ASN
1	B	54	GLN
1	B	57	HIS
1	B	247	GLN
1	B	250	ASN
1	B	382	GLN
1	B	387	GLN
1	B	422	ASN
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 oligosaccharides 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	$\# Z > 2$
5	BIB	A	505	-	5,6,6	0.90	0	5,7,7	0.91	0
5	BIB	B	1505	-	5,6,6	0.99	0	5,7,7	0.57	0
3	DTT	A	503	1	7,7,7	0.49	0	4,8,8	1.34	0
4	TRS	A	504	-	7,7,7	0.36	0	9,9,9	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BIB	A	505	-	-	4/6/6/6	-
5	BIB	B	1505	-	-	0/6/6/6	-
3	DTT	A	503	1	-	4/8/8/8	-
4	TRS	A	504	-	-	3/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	DTT	S1-C1-C2-O2
3	A	503	DTT	S1-C1-C2-C3
3	A	503	DTT	C2-C3-C4-S4
3	A	503	DTT	O3-C3-C4-S4
5	A	505	BIB	C5-C3-C4-N1
4	A	504	TRS	N-C-C1-O1
4	A	504	TRS	C2-C-C1-O1
4	A	504	TRS	C3-C-C1-O1
5	A	505	BIB	C2-C3-C4-N1
5	A	505	BIB	C4-C3-C5-O7
5	A	505	BIB	C4-C3-C5-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	430/463 (92%)	0.50	9 (2%) 63 54	14, 20, 24, 31	0
1	B	424/463 (91%)	0.71	23 (5%) 31 24	16, 20, 22, 29	0
All	All	854/926 (92%)	0.60	32 (3%) 45 36	14, 20, 23, 31	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	GLY	3.4
1	B	145	TYR	3.2
1	B	25	ALA	3.2
1	A	386	ASP	3.2
1	A	19	THR	3.0
1	B	455	HIS	2.8
1	A	41	GLU	2.7
1	B	310	ILE	2.5
1	B	454	GLY	2.5
1	B	303	ALA	2.5
1	A	190	GLY	2.4
1	B	106	GLY	2.4
1	A	192	ASP	2.4
1	B	54	GLN	2.4
1	B	109	THR	2.4
1	B	143	ASN	2.3
1	B	380	PHE	2.3
1	B	58	GLU	2.3
1	B	41	GLU	2.3
1	B	33	GLY	2.3
1	B	264	GLY	2.2
1	A	79	ASN	2.1
1	B	104	ASN	2.1
1	B	151	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	150	ASP	2.1
1	B	43	GLY	2.1
1	A	77	PHE	2.1
1	B	149	TYR	2.1
1	B	263	ALA	2.1
1	A	26	ALA	2.1
1	B	84	LEU	2.0
1	A	455	HIS	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(Å ²)	Q<0.9
4	TRS	A	504	8/8	0.70	0.17	19,20,20,20	0
5	BIB	A	505	7/7	0.72	0.14	15,18,18,18	0
5	BIB	B	1505	7/7	0.83	0.12	19,19,20,20	0
3	DTT	A	503	8/8	0.85	0.13	30,31,31,33	0
2	ZN	B	501	1/1	0.93	0.06	26,26,26,26	0
2	ZN	B	500	1/1	0.97	0.03	20,20,20,20	0
2	ZN	A	500	1/1	0.99	0.07	21,21,21,21	0
2	ZN	A	501	1/1	0.99	0.07	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.