Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:01 pm BST

PDB ID	:	1R43
Title	:	Crystal structure of beta-alanine synthase from Saccharomyces kluyveri (selenomethionine substituted protein)
Authors	:	Lundgren, S.; Gojkovic, Z.; Piskur, J.; Dobritzsch, 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 following versions of software and data (see references ⓘ) were used in the production of this report:

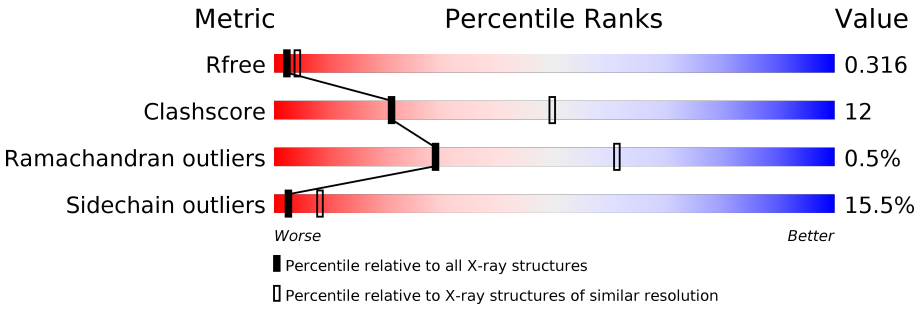
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	463	63% 26% 5% 5%
1	B	463	60% 28% 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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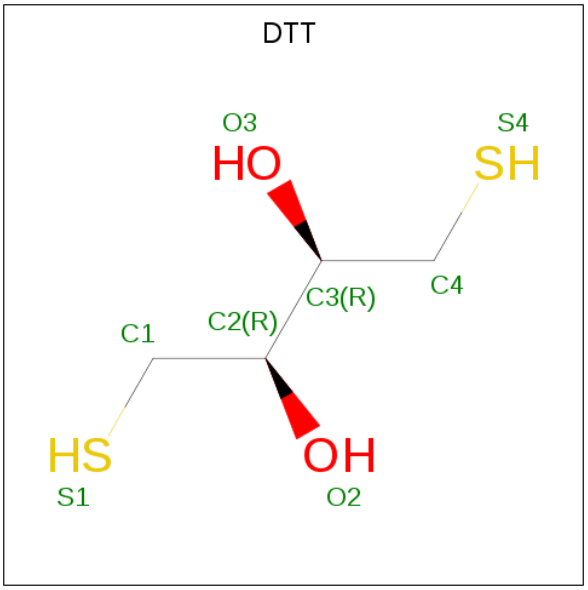
Chain	Residue	Modelled	Actual	Comment	Reference
B	410	MSE	MET	MODIFIED RESIDUE	UNP Q96W94
B	456	HIS	-	EXPRESSION TAG	UNP Q96W94
B	457	HIS	-	EXPRESSION TAG	UNP Q96W94
B	458	HIS	-	EXPRESSION TAG	UNP Q96W94
B	459	HIS	-	EXPRESSION TAG	UNP Q96W94
B	460	HIS	-	EXPRESSION TAG	UNP Q96W94
B	461	HIS	-	EXPRESSION 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 2 2	0	0
2	A	2	Total Zn 2 2	0	0

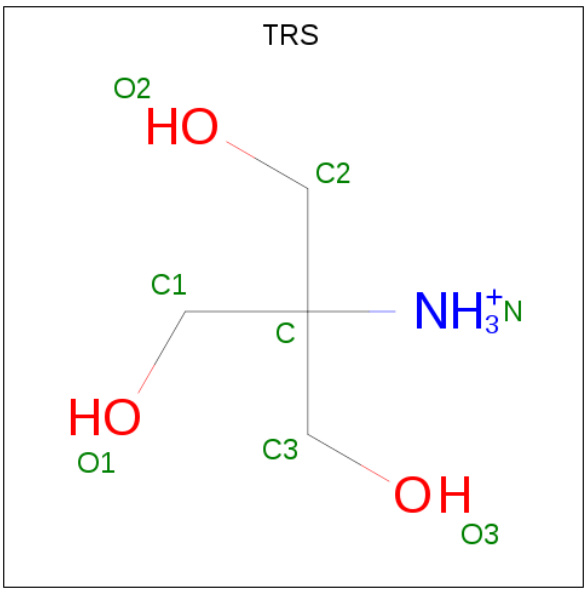
- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



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

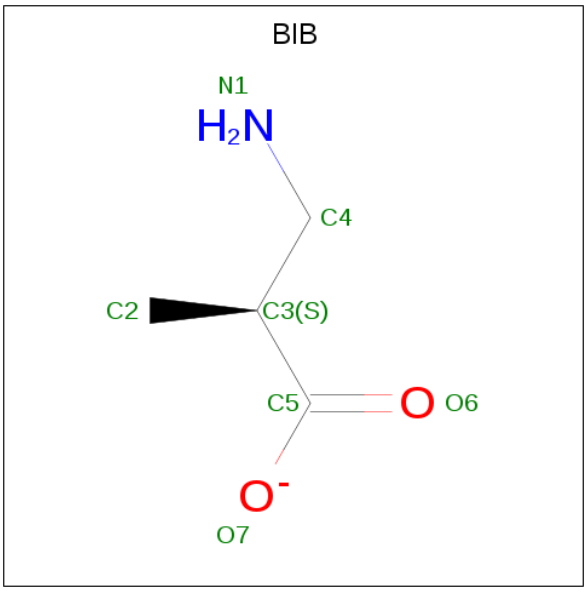
- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

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



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

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



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

- Molecule 6 is water.

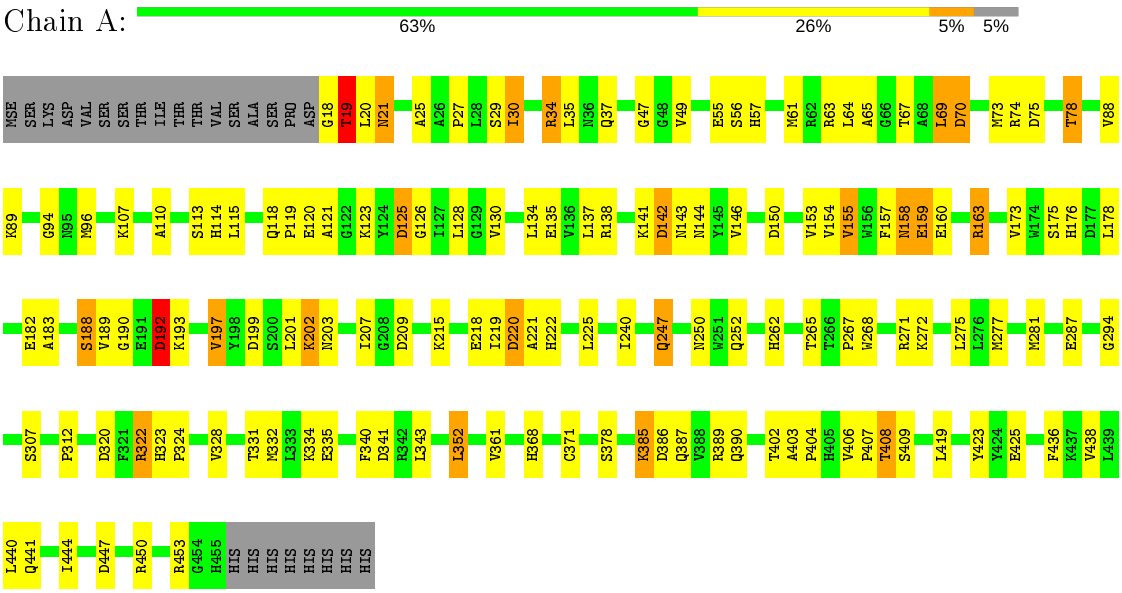
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	54	Total O 54 54	0	0
6	B	14	Total O 14 14	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

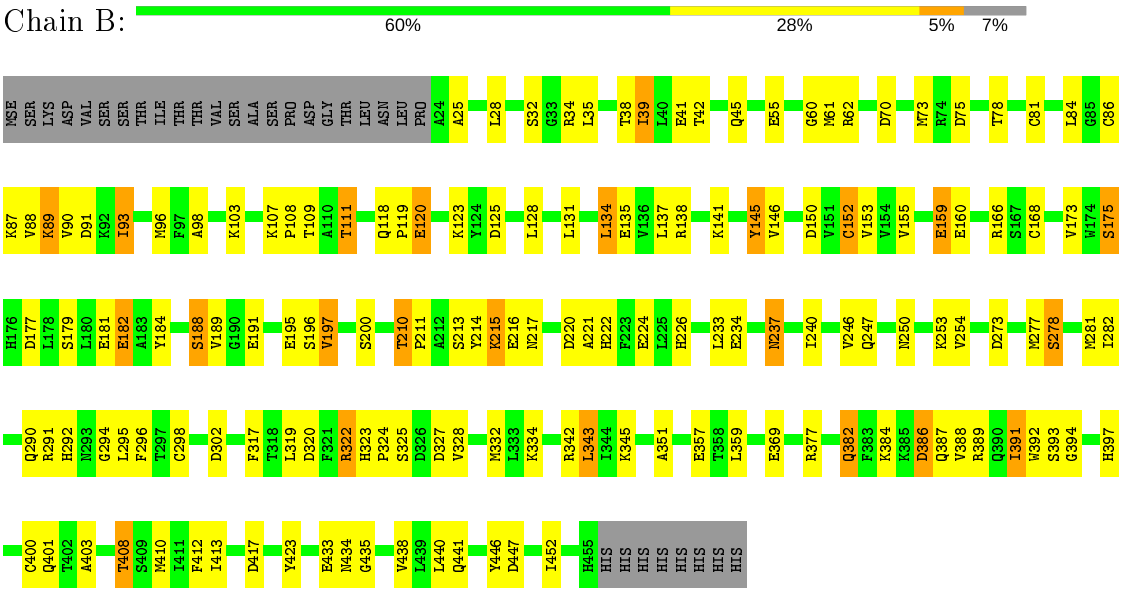
- Molecule 1: beta-alanine synthase

Chain A:



- Molecule 1: beta-alanine synthase

Chain B:



4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [1]	2.66 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.211 , 0.274 0.285 , 0.316	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 , 13.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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 (i)

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: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

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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: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

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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: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:135:GLU:HA	1:B:138:ARG:HB2	1.92	0.50
1:B:96:MSE:HB2	1:B:155:VAL:HG12	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: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: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: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: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

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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:163:ARG:O	1:A:188:SER:HA	2.15	0.45
1:A:74:ARG:HH22	1:A:157:PHE:HA	1.81	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: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:B:434:ASN:O	1:B:438:VAL:HG23	2.18	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: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: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:221:ALA:HB2	1:B:446:TYR:CZ	2.53	0.43
1:B:78:THR:HG23	1:B:96:MSE:CE	2.48	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: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

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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: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:18:GLY:O	1:A:19:THR:C	2.58	0.42
1:A:70:ASP:O	1:A:74:ARG:HG3	2.20	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
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: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:272:LYS:HB3	1:A:352:LEU:HD22	2.03	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:B:296:PHE:HE1	1:B:319:LEU:HD22	1.84	0.41
1:A:440:LEU:O	1:A:444:ILE:HG13	2.21	0.41
1:B:210:THR:HA	1:B:211:PRO:HD3	1.96	0.41
1:B:38:THR:HG22	1:B:131:LEU:HD13	2.02	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 (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	436/463 (94%)	404 (93%)	30 (7%)	2 (0%)	29 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	430/463 (93%)	395 (92%)	33 (8%)	2 (0%)	29 61
All	All	866/926 (94%)	799 (92%)	63 (7%)	4 (0%)	29 61

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 (i)

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%)	3 11
1	B	355/375 (95%)	294 (83%)	61 (17%)	2 6
All	All	715/750 (95%)	604 (84%)	111 (16%)	2 8

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

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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

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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

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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 (i)

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	B	1505	-	2,6,6	0.55	0	0,7,7	0.00	-
5	BIB	A	505	-	2,6,6	0.49	0	0,7,7	0.00	-
4	TRS	A	504	-	7,7,7	0.34	0	9,9,9	0.53	0
3	DTT	A	503	1	7,7,7	0.49	0	4,8,8	1.30	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	B	1505	-	-	0/1/6/6	-
5	BIB	A	505	-	-	1/1/6/6	-
4	TRS	A	504	-	-	3/9/9/9	-
3	DTT	A	503	1	-	4/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) 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
4	A	504	TRS	N-C-C1-O1
4	A	504	TRS	C2-C-C1-O1
4	A	504	TRS	C3-C-C1-O1

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Mol	Chain	Res	Type	Atoms
5	A	505	BIB	C2-C3-C4-N1

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.