



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 10:30 AM GMT

PDB ID : 1R3N
Title : Crystal structure of beta-alanine synthase from *Saccharomyces kluyveri*
Authors : Lundgren, S.; Gojkovic, Z.; Piskur, J.; Dobritsch, D.
Deposited on : 2003-10-02
Resolution : 2.70 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

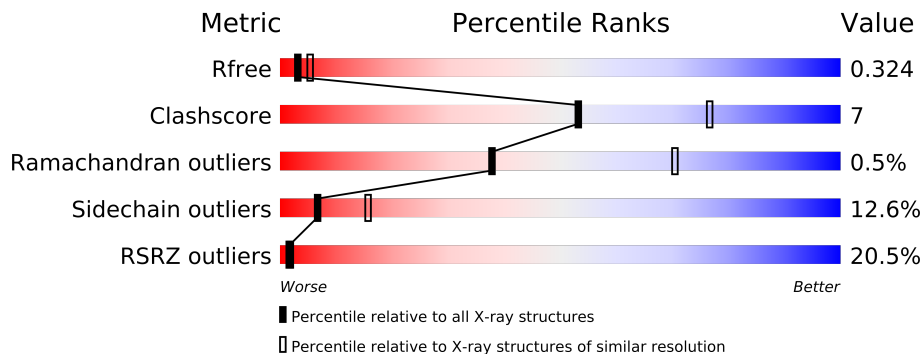
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	462	
1	B	462	
1	C	462	
1	D	462	
1	E	462	
1	F	462	
1	G	462	
1	H	462	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	BIB	C	3502	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	BIB	E	6502	-	X
3	BIB	G	8502	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27487 atoms, of which 0 are hydrogen and 0 are deuterium.

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	0	0	0
			3379	2130	580	653	16			
1	B	433	Total	C	N	O	S	0	0	0
			3344	2108	574	646	16			
1	C	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			
1	D	437	Total	C	N	O	S	0	0	0
			3375	2128	579	652	16			
1	E	433	Total	C	N	O	S	0	0	0
			3344	2108	574	646	16			
1	F	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			
1	G	430	Total	C	N	O	S	0	0	0
			3327	2097	571	643	16			
1	H	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	461	HIS	-	EXPRESSION TAG	UNP Q96W94
B	462	HIS	-	EXPRESSION TAG	UNP Q96W94
B	463	HIS	-	EXPRESSION TAG	UNP Q96W94
C	456	HIS	-	EXPRESSION TAG	UNP Q96W94
C	457	HIS	-	EXPRESSION TAG	UNP Q96W94
C	458	HIS	-	EXPRESSION TAG	UNP Q96W94
C	459	HIS	-	EXPRESSION TAG	UNP Q96W94
C	460	HIS	-	EXPRESSION TAG	UNP Q96W94
C	461	HIS	-	EXPRESSION TAG	UNP Q96W94
C	462	HIS	-	EXPRESSION TAG	UNP Q96W94
C	463	HIS	-	EXPRESSION TAG	UNP Q96W94
D	456	HIS	-	EXPRESSION TAG	UNP Q96W94
D	457	HIS	-	EXPRESSION TAG	UNP Q96W94
D	458	HIS	-	EXPRESSION TAG	UNP Q96W94
D	459	HIS	-	EXPRESSION TAG	UNP Q96W94
D	460	HIS	-	EXPRESSION TAG	UNP Q96W94
D	461	HIS	-	EXPRESSION TAG	UNP Q96W94
D	462	HIS	-	EXPRESSION TAG	UNP Q96W94
D	463	HIS	-	EXPRESSION TAG	UNP Q96W94
E	456	HIS	-	EXPRESSION TAG	UNP Q96W94
E	457	HIS	-	EXPRESSION TAG	UNP Q96W94
E	458	HIS	-	EXPRESSION TAG	UNP Q96W94
E	459	HIS	-	EXPRESSION TAG	UNP Q96W94
E	460	HIS	-	EXPRESSION TAG	UNP Q96W94
E	461	HIS	-	EXPRESSION TAG	UNP Q96W94
E	462	HIS	-	EXPRESSION TAG	UNP Q96W94
E	463	HIS	-	EXPRESSION TAG	UNP Q96W94
F	456	HIS	-	EXPRESSION TAG	UNP Q96W94
F	457	HIS	-	EXPRESSION TAG	UNP Q96W94
F	458	HIS	-	EXPRESSION TAG	UNP Q96W94
F	459	HIS	-	EXPRESSION TAG	UNP Q96W94
F	460	HIS	-	EXPRESSION TAG	UNP Q96W94
F	461	HIS	-	EXPRESSION TAG	UNP Q96W94
F	462	HIS	-	EXPRESSION TAG	UNP Q96W94
F	463	HIS	-	EXPRESSION TAG	UNP Q96W94
G	456	HIS	-	EXPRESSION TAG	UNP Q96W94
G	457	HIS	-	EXPRESSION TAG	UNP Q96W94
G	458	HIS	-	EXPRESSION TAG	UNP Q96W94
G	459	HIS	-	EXPRESSION TAG	UNP Q96W94
G	460	HIS	-	EXPRESSION TAG	UNP Q96W94
G	461	HIS	-	EXPRESSION TAG	UNP Q96W94
G	462	HIS	-	EXPRESSION TAG	UNP Q96W94

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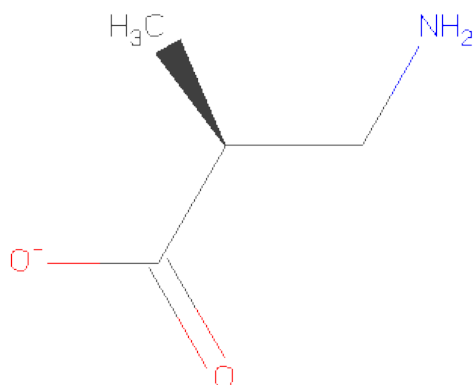
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Chain	Residue	Modelled	Actual	Comment	Reference
G	463	HIS	-	EXPRESSION TAG	UNP Q96W94
H	456	HIS	-	EXPRESSION TAG	UNP Q96W94
H	457	HIS	-	EXPRESSION TAG	UNP Q96W94
H	458	HIS	-	EXPRESSION TAG	UNP Q96W94
H	459	HIS	-	EXPRESSION TAG	UNP Q96W94
H	460	HIS	-	EXPRESSION TAG	UNP Q96W94
H	461	HIS	-	EXPRESSION TAG	UNP Q96W94
H	462	HIS	-	EXPRESSION TAG	UNP Q96W94
H	463	HIS	-	EXPRESSION TAG	UNP Q96W94

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is BETA-AMINO ISOBUTYRATE (three-letter code: BIB) (formula: C₄H₈NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			7	4	1	2		
3	A	1	Total	C	N	O	0	0
			7	4	1	2		
3	C	1	Total	C	N	O	0	0
			7	4	1	2		
3	D	1	Total	C	N	O	0	0
			7	4	1	2		
3	E	1	Total	C	N	O	0	0
			7	4	1	2		
3	E	1	Total	C	N	O	0	0
			7	4	1	2		
3	G	1	Total	C	N	O	0	0
			7	4	1	2		
3	G	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 4 is water.

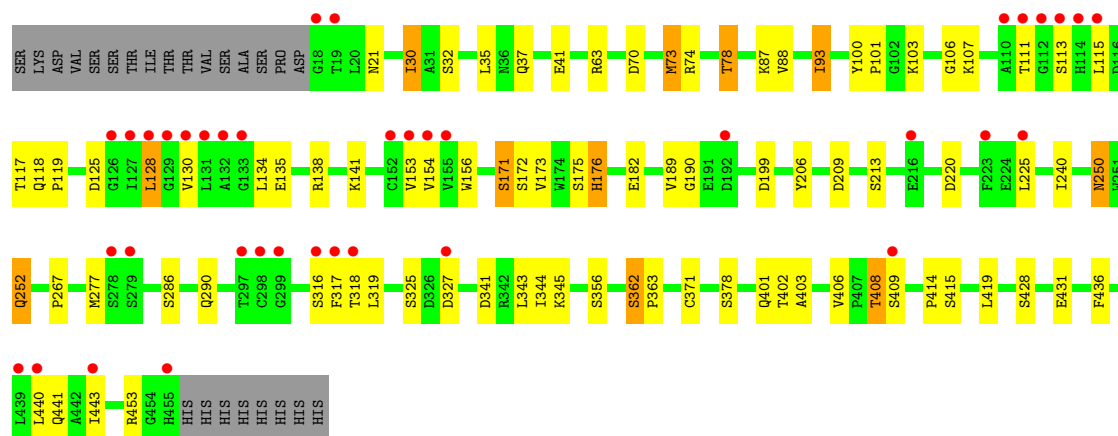
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	60	Total	O	0	0
			60	60		
4	C	91	Total	O	0	0
			91	91		
4	D	54	Total	O	0	0
			54	54		

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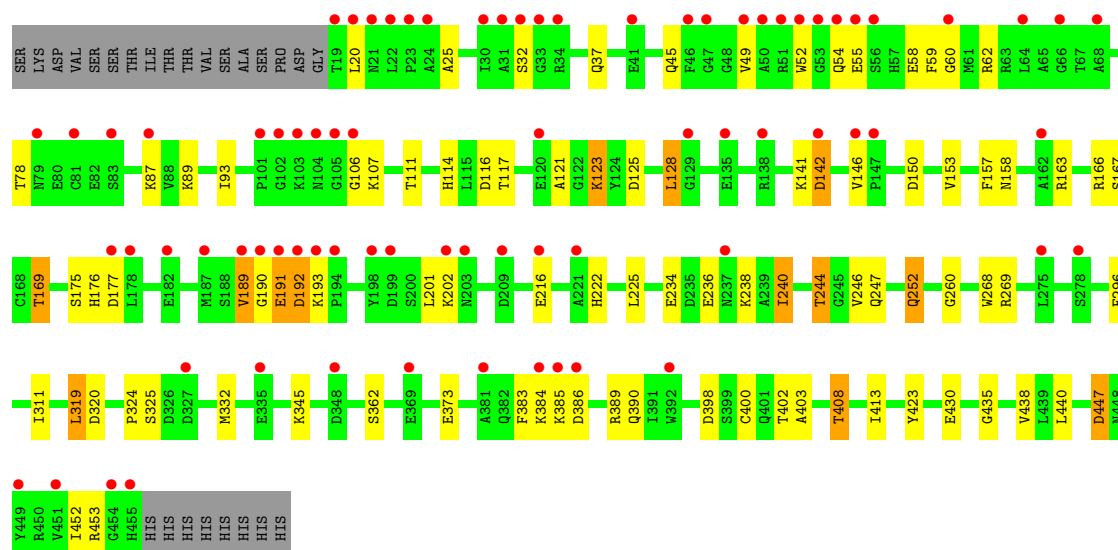
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	20	Total 20	O 20	0	0
4	F	101	Total 101	O 101	0	0
4	G	24	Total 24	O 24	0	0
4	H	50	Total 50	O 50	0	0

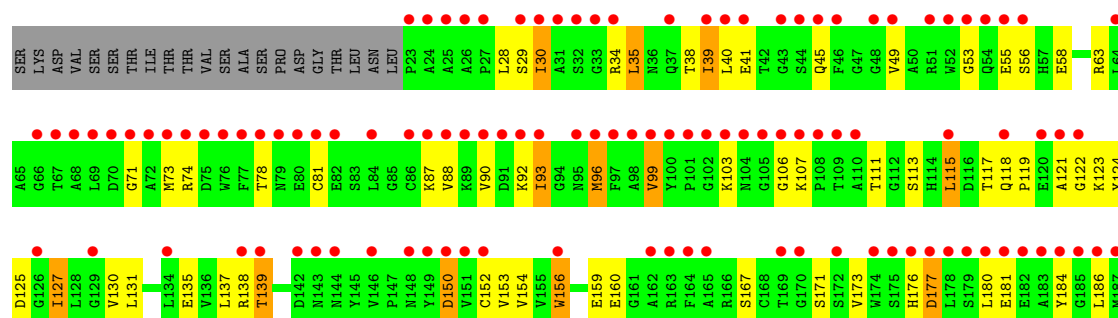
Chain C: 

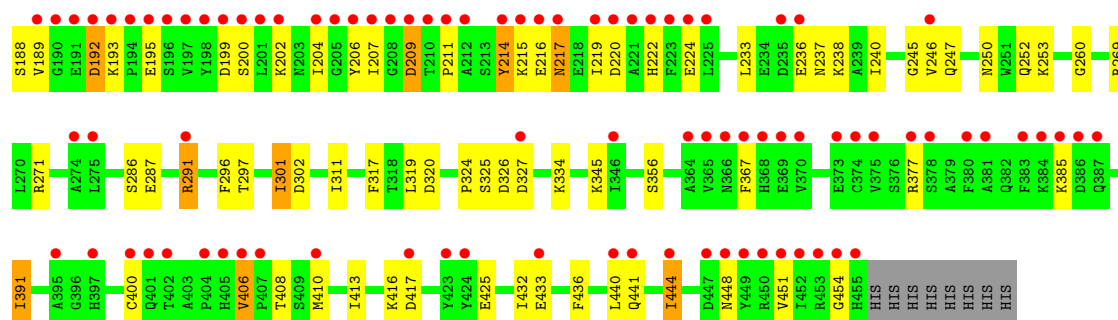


Chain D: 



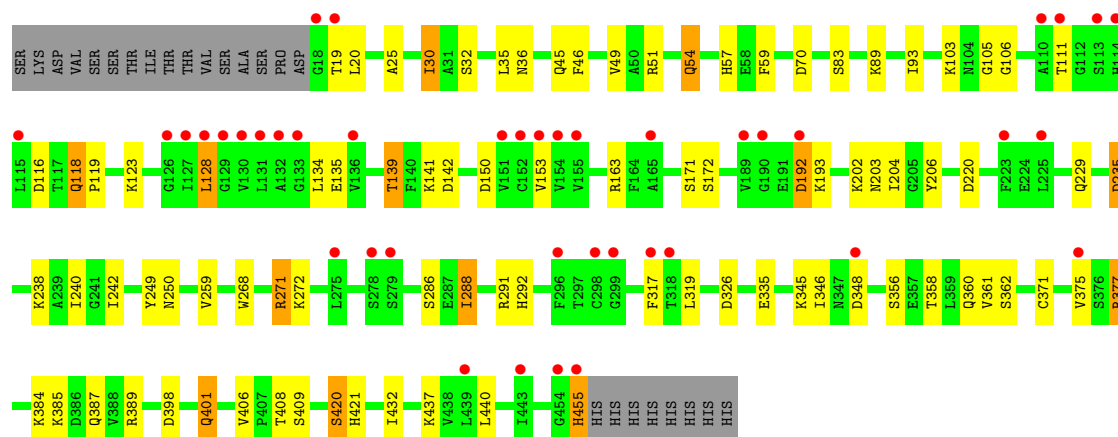
Chain E:





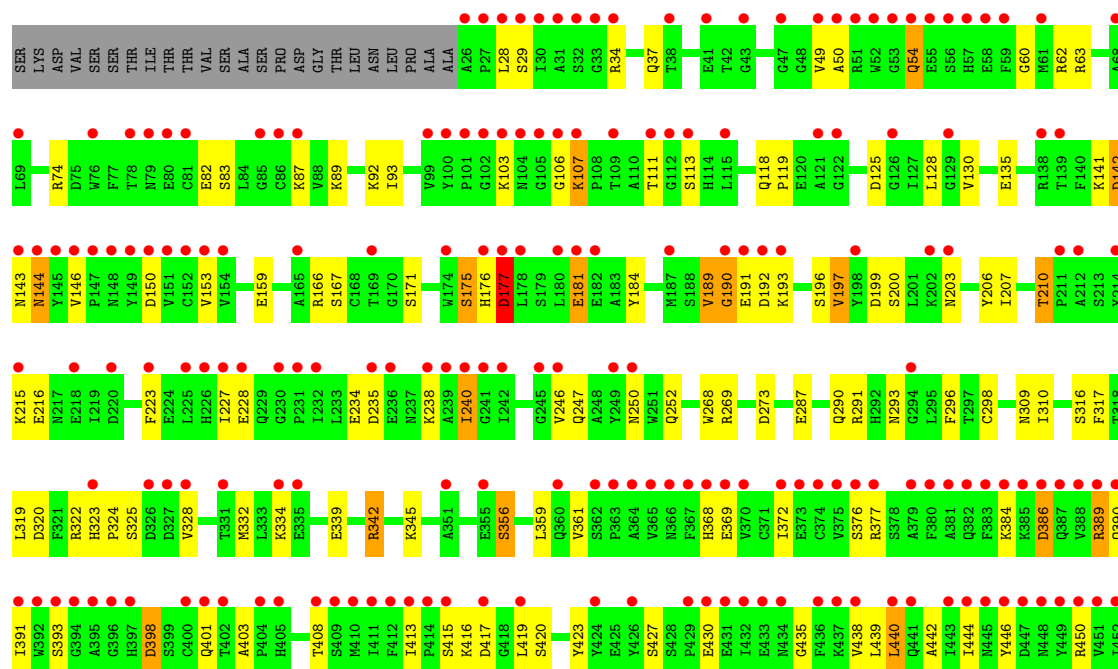
• Molecule 1: beta-alanine synthase

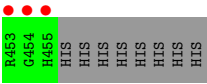
Chain F:



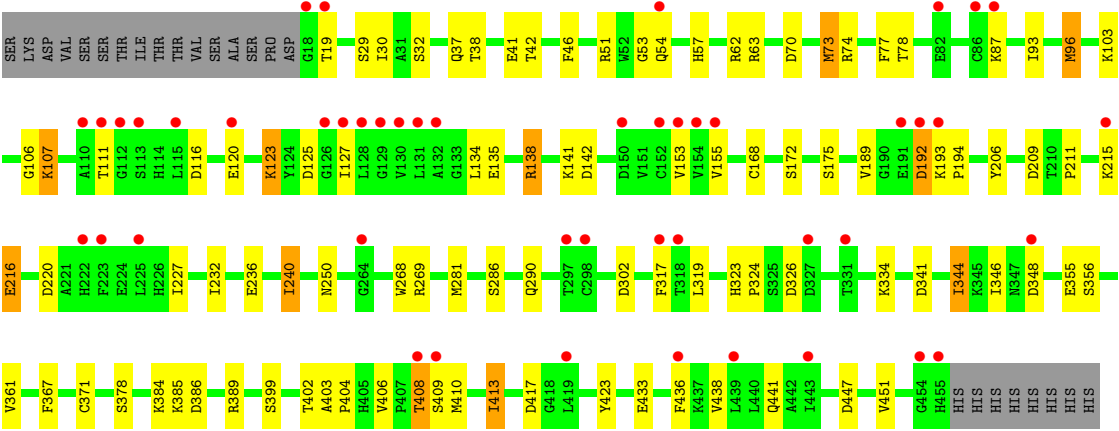
• Molecule 1: beta-alanine synthase

Chain G:





• 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	117.23Å 77.12Å 225.52Å 90.00° 95.05° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 24.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (25.00-2.70) 95.9 (24.90-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.208 , 0.266 0.292 , 0.324	Depositor DCC
R_{free} test set	5290 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	10 of 106175 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	27487	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.92 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5506e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

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	0.56	1/3457 (0.0%)	0.80	15/4689 (0.3%)
1	B	0.43	0/3422	0.75	14/4640 (0.3%)
1	C	0.52	0/3457	0.75	6/4689 (0.1%)
1	D	0.44	0/3453	0.73	8/4684 (0.2%)
1	E	0.39	0/3422	0.71	10/4640 (0.2%)
1	F	0.49	0/3457	0.73	7/4689 (0.1%)
1	G	0.38	0/3404	0.72	13/4615 (0.3%)
1	H	0.44	0/3457	0.74	12/4689 (0.3%)
All	All	0.46	1/27529 (0.0%)	0.74	85/37335 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLY	C-O	-9.59	1.08	1.23

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	125	ASP	CB-CG-OD2	9.55	126.90	118.30
1	B	125	ASP	CB-CG-OD2	8.89	126.30	118.30
1	A	105	GLY	CA-C-N	8.52	133.25	116.20
1	D	125	ASP	CB-CG-OD2	7.93	125.44	118.30
1	A	309	ASN	CB-CA-C	-7.89	94.61	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3379	0	3264	49	0
1	B	3344	0	3227	39	1
1	C	3379	0	3264	44	0
1	D	3375	0	3261	39	0
1	E	3344	0	3227	73	0
1	F	3379	0	3264	41	0
1	G	3327	0	3209	51	1
1	H	3379	0	3264	44	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	7	0	8	1	0
3	B	7	0	8	0	0
3	C	7	0	8	0	0
3	D	7	0	8	0	0
3	E	14	0	16	0	0
3	G	14	0	16	0	0
4	A	109	0	0	4	0
4	B	60	0	0	3	0
4	C	91	0	0	2	0
4	D	54	0	0	3	0
4	E	20	0	0	0	0
4	F	101	0	0	3	0
4	G	24	0	0	3	0
4	H	50	0	0	2	0
All	All	27487	0	26044	370	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 370 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:189:VAL:HG23	1:D:190:GLY:H	1.24	1.03
1:E:118:GLN:HG3	1:E:119:PRO:HD2	1.47	0.96
1:E:71:GLY:HA3	1:E:204:ILE:CG2	1.97	0.94
1:H:346:ILE:HD11	4:H:511:HOH:O	1.68	0.93
1:B:55:GLU:HB2	1:B:58:GLU:HG3	1.49	0.90

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:293:ASN:ND2	1:G:144:ASN:O[1_565]	1.98	0.22

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	436/462 (94%)	420 (96%)	16 (4%)	0	100	100
1	B	431/462 (93%)	418 (97%)	11 (3%)	2 (0%)	38	70
1	C	436/462 (94%)	420 (96%)	14 (3%)	2 (0%)	38	70
1	D	435/462 (94%)	419 (96%)	12 (3%)	4 (1%)	25	55
1	E	431/462 (93%)	417 (97%)	12 (3%)	2 (0%)	38	70
1	F	436/462 (94%)	422 (97%)	12 (3%)	2 (0%)	38	70
1	G	428/462 (93%)	411 (96%)	13 (3%)	4 (1%)	25	55
1	H	436/462 (94%)	422 (97%)	13 (3%)	1 (0%)	56	86
All	All	3469/3696 (94%)	3349 (96%)	103 (3%)	17 (0%)	38	70

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	20	LEU
1	B	106	GLY
1	B	454	GLY
1	C	21	ASN

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Mol	Chain	Res	Type
1	C	106	GLY

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	360/383 (94%)	323 (90%)	37 (10%)	10	23
1	B	356/383 (93%)	314 (88%)	42 (12%)	8	18
1	C	360/383 (94%)	332 (92%)	28 (8%)	18	40
1	D	360/383 (94%)	317 (88%)	43 (12%)	8	18
1	E	356/383 (93%)	284 (80%)	72 (20%)	2	5
1	F	360/383 (94%)	321 (89%)	39 (11%)	9	21
1	G	355/383 (93%)	289 (81%)	66 (19%)	2	6
1	H	360/383 (94%)	325 (90%)	35 (10%)	12	27
All	All	2867/3064 (94%)	2505 (87%)	362 (13%)	7	16

5 of 362 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	92	LYS
1	E	253	LYS
1	H	107	LYS
1	E	107	LYS
1	E	180	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	247	GLN
1	E	247	GLN
1	G	405	HIS
1	D	250	ASN
1	D	360	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	BIB	A	2502	-	4,6,6	1.06	0	4,7,7	2.24	1 (25%)
3	BIB	B	1502	-	4,6,6	0.58	0	4,7,7	2.41	2 (50%)
3	BIB	C	3502	-	4,6,6	0.50	0	4,7,7	5.72	1 (25%)
3	BIB	D	4502	-	4,6,6	0.48	0	4,7,7	14.00	2 (50%)
3	BIB	E	5502	-	4,6,6	0.51	0	4,7,7	15.06	1 (25%)
3	BIB	E	6502	-	4,6,6	1.13	1 (25%)	4,7,7	5.00	1 (25%)
3	BIB	G	7502	-	4,6,6	0.42	0	4,7,7	0.52	0
3	BIB	G	8502	-	4,6,6	0.85	0	4,7,7	11.30	1 (25%)

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	BIB	A	2502	-	-	0/2/6/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BIB	B	1502	-	-	0/2/6/6	0/0/0/0
3	BIB	C	3502	-	-	0/2/6/6	0/0/0/0
3	BIB	D	4502	-	-	0/2/6/6	0/0/0/0
3	BIB	E	5502	-	-	0/2/6/6	0/0/0/0
3	BIB	E	6502	-	-	0/2/6/6	0/0/0/0
3	BIB	G	7502	-	-	0/2/6/6	0/0/0/0
3	BIB	G	8502	-	-	0/2/6/6	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	6502	BIB	C4-C3	2.08	1.55	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5502	BIB	C4-C3-C5	-30.07	108.46	111.91
3	D	4502	BIB	C4-C3-C5	-27.92	108.71	111.91
3	G	8502	BIB	C4-C3-C5	22.60	114.50	111.91
3	C	3502	BIB	C4-C3-C5	-11.37	110.61	111.91
3	E	6502	BIB	C4-C3-C5	9.96	113.05	111.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	438/462 (94%)	0.86	54 (12%) 5 5	12, 16, 19, 29	0
1	B	433/462 (93%)	1.02	66 (15%) 3 3	13, 16, 18, 20	0
1	C	438/462 (94%)	0.71	38 (8%) 10 10	13, 16, 19, 30	0
1	D	437/462 (94%)	1.12	77 (17%) 2 2	14, 16, 17, 20	0
1	E	433/462 (93%)	2.20	198 (45%) 1 0	15, 16, 17, 20	0
1	F	438/462 (94%)	0.67	41 (9%) 9 8	13, 16, 19, 31	0
1	G	430/462 (93%)	2.08	195 (45%) 1 0	13, 16, 17, 20	0
1	H	438/462 (94%)	0.81	47 (10%) 6 6	12, 16, 19, 24	0
All	All	3485/3696 (94%)	1.18	716 (20%) 1 2	12, 16, 18, 31	0

The worst 5 of 716 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	211	PRO	9.2
1	E	176	HIS	8.6
1	B	455	HIS	8.3
1	E	455	HIS	8.0
1	G	53	GLY	7.7

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	BIB	E	6502	7/7	0.28	4.79	21,22,24,24	0
3	BIB	G	8502	7/7	0.30	3.20	19,21,21,22	0
3	BIB	C	3502	7/7	0.26	2.40	24,26,27,27	0
3	BIB	E	5502	7/7	0.30	1.58	16,17,18,18	0
3	BIB	D	4502	7/7	0.22	0.27	16,16,17,17	0
3	BIB	G	7502	7/7	0.34	0.24	12,13,15,15	0
3	BIB	A	2502	7/7	0.20	0.09	15,19,21,21	0
3	BIB	B	1502	7/7	0.21	-0.60	19,23,24,25	0
2	ZN	A	500	1/1	0.21	-0.72	15,15,15,15	0
2	ZN	F	500	1/1	0.18	-1.01	16,16,16,16	0
2	ZN	C	500	1/1	0.18	-1.06	16,16,16,16	0
2	ZN	H	500	1/1	0.15	-1.40	15,15,15,15	0
2	ZN	C	501	1/1	0.14	-1.42	18,18,18,18	0
2	ZN	B	500	1/1	0.12	-1.70	16,16,16,16	0
2	ZN	A	501	1/1	0.15	-1.71	18,18,18,18	0
2	ZN	F	501	1/1	0.13	-1.77	18,18,18,18	0
2	ZN	H	501	1/1	0.13	-1.90	18,18,18,18	0
2	ZN	G	501	1/1	0.14	-2.36	17,17,17,17	0
2	ZN	E	500	1/1	0.07	-2.48	16,16,16,16	0
2	ZN	B	501	1/1	0.05	-2.89	18,18,18,18	0
2	ZN	D	500	1/1	0.08	-2.92	15,15,15,15	0
2	ZN	G	500	1/1	0.06	-3.02	15,15,15,15	0
2	ZN	D	501	1/1	0.07	-3.65	18,18,18,18	0
2	ZN	E	501	1/1	0.08	-3.74	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.