wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2024 – 12:09 PM EST

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

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

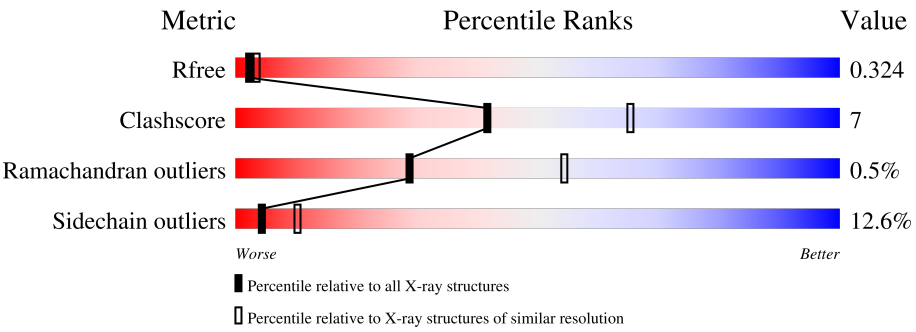
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	462	73% 19% • 5%
1	B	462	71% 21% • 6%
1	C	462	76% 16% • 5%
1	D	462	75% 17% • 5%
1	E	462	64% 26% 5% 6%
1	F	462	76% 16% • 5%
1	G	462	65% 24% • 7%

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Mol	Chain	Length	Quality of chain
1	H	462	73% 19% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27487 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
			Total	C	N	O	S			
1	A	438	3379	2130	580	653	16	0	0	0
1	B	433	3344	2108	574	646	16	0	0	0
1	C	438	3379	2130	580	653	16	0	0	0
1	D	437	3375	2128	579	652	16	0	0	0
1	E	433	3344	2108	574	646	16	0	0	0
1	F	438	3379	2130	580	653	16	0	0	0
1	G	430	3327	2097	571	643	16	0	0	0
1	H	438	3379	2130	580	653	16	0	0	0

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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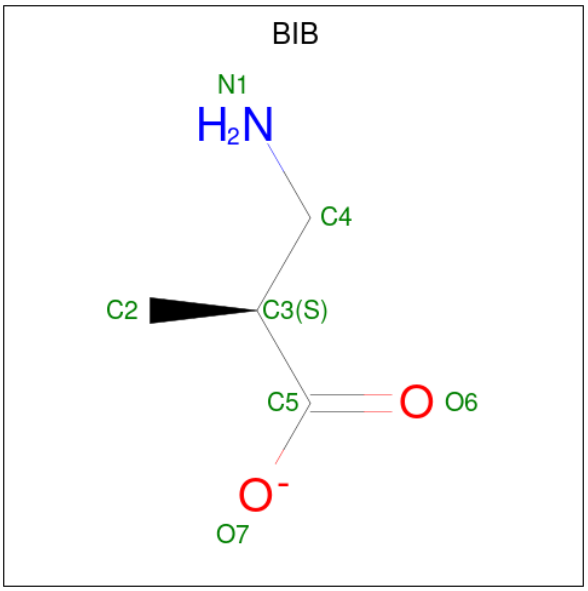
Chain	Residue	Modelled	Actual	Comment	Reference
G	463	HIS	-	expression tag	UNP Q96W94
H	456	HIS	-	expression tag	UNP Q96W94
H	457	HIS	-	expression tag	UNP Q96W94
H	458	HIS	-	expression tag	UNP Q96W94
H	459	HIS	-	expression tag	UNP Q96W94
H	460	HIS	-	expression tag	UNP Q96W94
H	461	HIS	-	expression tag	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
			Total	Zn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0
2	E	2	2	2	0	0
2	F	2	2	2	0	0
2	G	2	2	2	0	0
2	H	2	2	2	0	0

- Molecule 3 is BETA-AMINO ISOBUTYRATE (three-letter code: BIB) (formula: $C_4H_8NO_2$).



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

- Molecule 4 is water.

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

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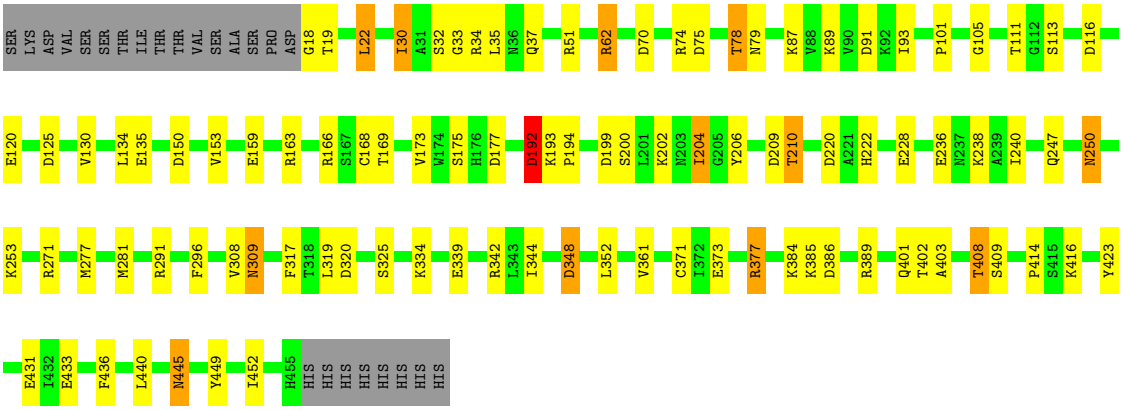
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	20	Total O 20 20	0	0
4	F	101	Total O 101 101	0	0
4	G	24	Total O 24 24	0	0
4	H	50	Total O 50 50	0	0

3 Residue-property plots (i)

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. 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.

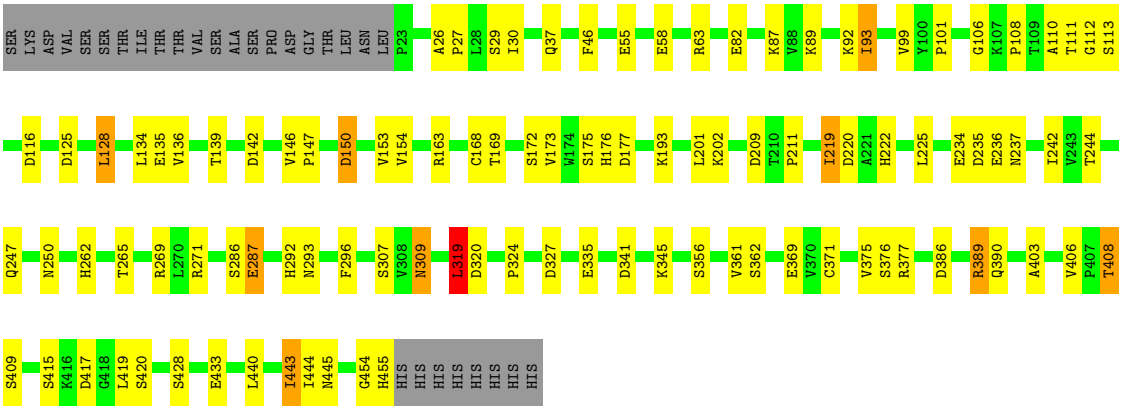
- Molecule 1: beta-alanine synthase

Chain A:



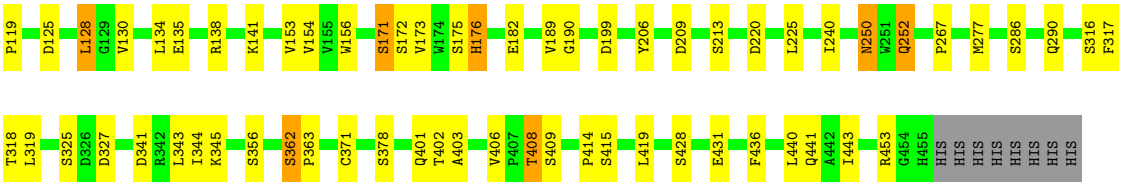
- Molecule 1: beta-alanine synthase

Chain B:



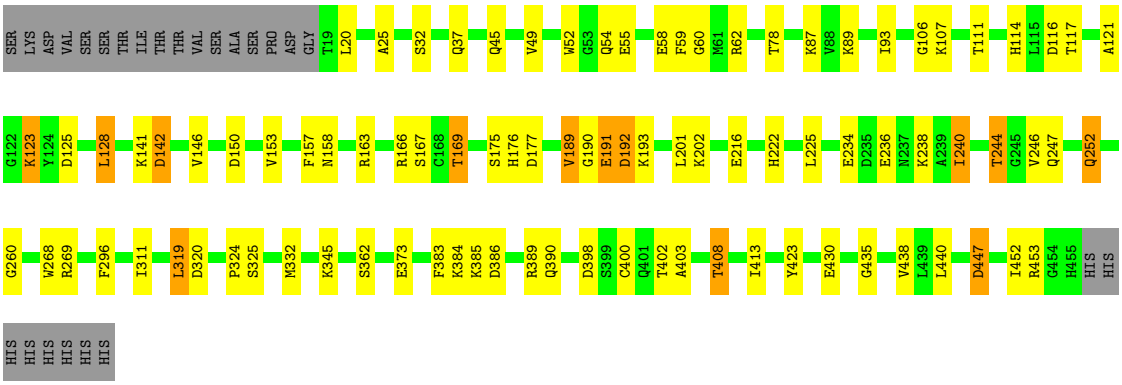
- Molecule 1: beta-alanine synthase

Chain C:



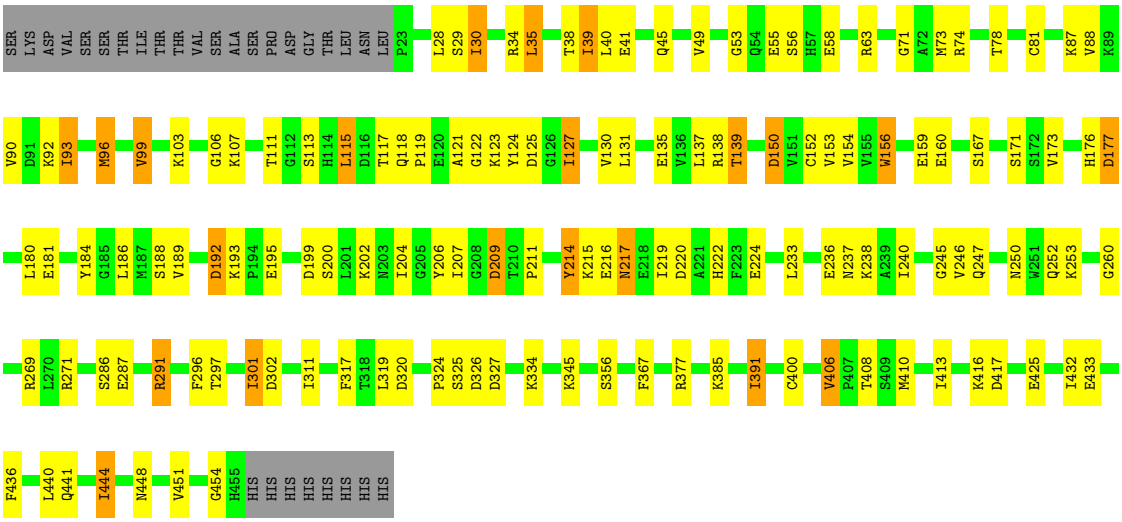
- Molecule 1: beta-alanine synthase

Chain D:



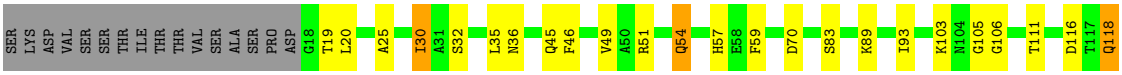
- Molecule 1: beta-alanine synthase

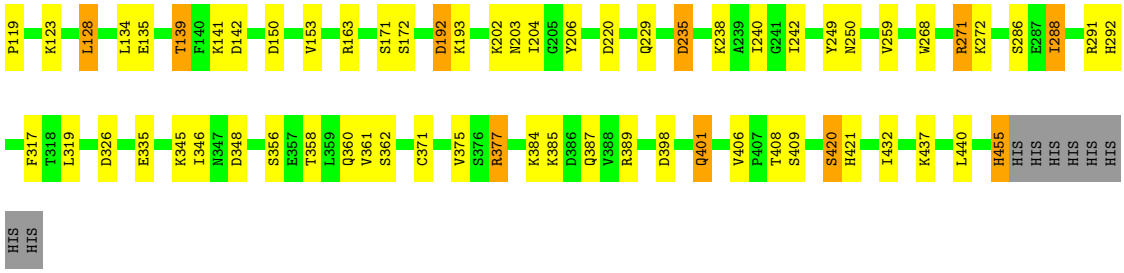
Chain E:



- Molecule 1: beta-alanine synthase

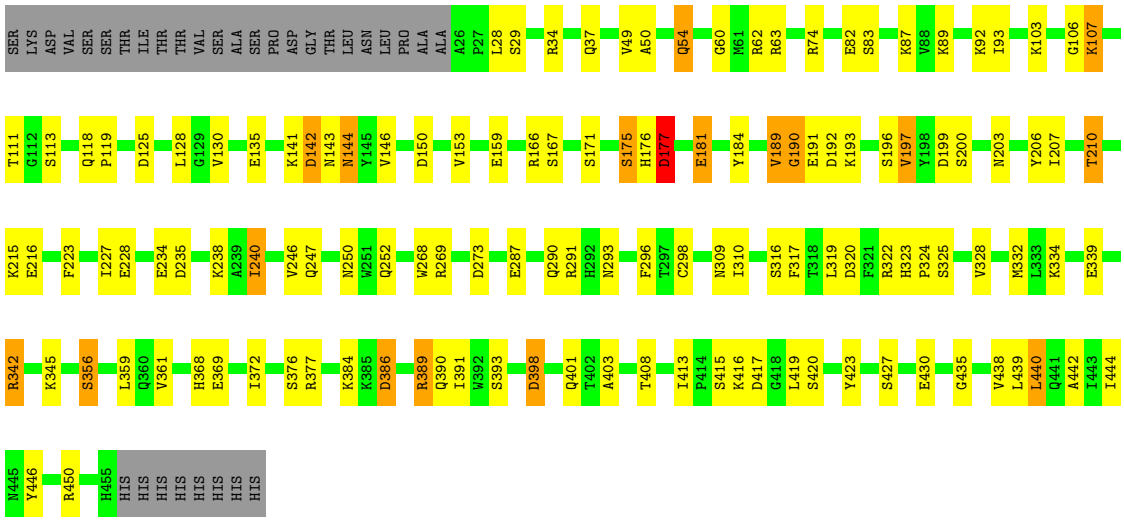
Chain F:





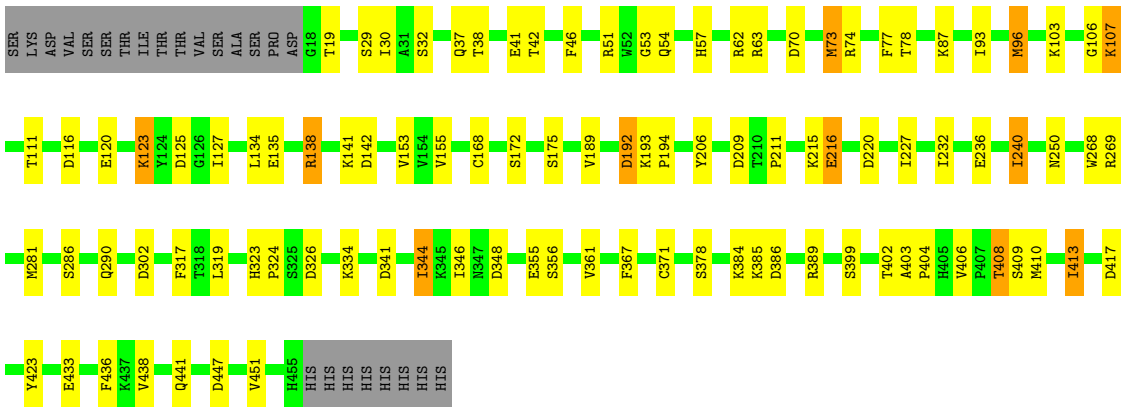
• Molecule 1: beta-alanine synthase

Chain G:



• Molecule 1: beta-alanine synthase

Chain H:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	5296 reflections (4.99%)	wwPDB-VP
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 , 19.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[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 (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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 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	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

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 7.

The worst 5 of 370 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: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	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:ND2	1:G:144:ASN:O[1_565]	1.98	0.22

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	436/462 (94%)	420 (96%)	16 (4%)	0	100	100
1	B	431/462 (93%)	418 (97%)	11 (3%)	2 (0%)	29	54
1	C	436/462 (94%)	420 (96%)	14 (3%)	2 (0%)	29	54
1	D	435/462 (94%)	419 (96%)	12 (3%)	4 (1%)	17	40
1	E	431/462 (93%)	417 (97%)	12 (3%)	2 (0%)	29	54
1	F	436/462 (94%)	422 (97%)	12 (3%)	2 (0%)	29	54
1	G	428/462 (93%)	411 (96%)	13 (3%)	4 (1%)	17	40
1	H	436/462 (94%)	422 (97%)	13 (3%)	1 (0%)	47	73
All	All	3469/3696 (94%)	3349 (96%)	103 (3%)	17 (0%)	29	54

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	20	LEU

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

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	360/383 (94%)	323 (90%)	37 (10%)	7 16
1	B	356/383 (93%)	314 (88%)	42 (12%)	5 12
1	C	360/383 (94%)	332 (92%)	28 (8%)	12 29
1	D	360/383 (94%)	317 (88%)	43 (12%)	5 12
1	E	356/383 (93%)	284 (80%)	72 (20%)	1 3
1	F	360/383 (94%)	321 (89%)	39 (11%)	6 15
1	G	355/383 (93%)	289 (81%)	66 (19%)	1 4
1	H	360/383 (94%)	325 (90%)	35 (10%)	8 19
All	All	2867/3064 (94%)	2505 (87%)	362 (13%)	4 10

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

Mol	Chain	Res	Type
1	F	103	LYS
1	G	200	SER
1	F	192	ASP
1	F	455	HIS
1	G	293	ASN

Sometimes 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	252	GLN

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Mol	Chain	Res	Type
1	G	434	ASN
1	E	397	HIS
1	G	405	HIS
1	G	118	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	G	8502	-	5,6,6	1.00	0	4,7,7	1.04	0
3	BIB	G	7502	-	5,6,6	0.90	0	4,7,7	0.93	0
3	BIB	B	1502	-	5,6,6	1.02	0	4,7,7	1.20	0
3	BIB	A	2502	-	5,6,6	0.99	0	4,7,7	0.79	0
3	BIB	D	4502	-	5,6,6	0.98	0	4,7,7	0.92	0
3	BIB	E	6502	-	5,6,6	0.87	0	4,7,7	1.19	0
3	BIB	C	3502	-	5,6,6	1.01	0	4,7,7	1.05	0
3	BIB	E	5502	-	5,6,6	1.01	0	4,7,7	0.76	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	BIB	G	8502	-	-	0/5/6/6	-
3	BIB	G	7502	-	-	0/5/6/6	-
3	BIB	B	1502	-	-	1/5/6/6	-
3	BIB	A	2502	-	-	0/5/6/6	-
3	BIB	D	4502	-	-	0/5/6/6	-
3	BIB	E	6502	-	-	2/5/6/6	-
3	BIB	C	3502	-	-	0/5/6/6	-
3	BIB	E	5502	-	-	0/5/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	6502	BIB	C4-C3-C5-O7
3	E	6502	BIB	C4-C3-C5-O6
3	B	1502	BIB	C2-C3-C4-N1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2502	BIB	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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