



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2023 – 07:12 pm GMT

PDB ID : 2V8G  
Title : Crystal structure of beta-alanine synthase from *Saccharomyces kluyveri* in complex with the product beta-alanine  
Authors : Lundgren, S.; Andersen, B.; Piskur, J.; Dobritzsch, D.  
Deposited on : 2007-08-07  
Resolution : 2.50 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, 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

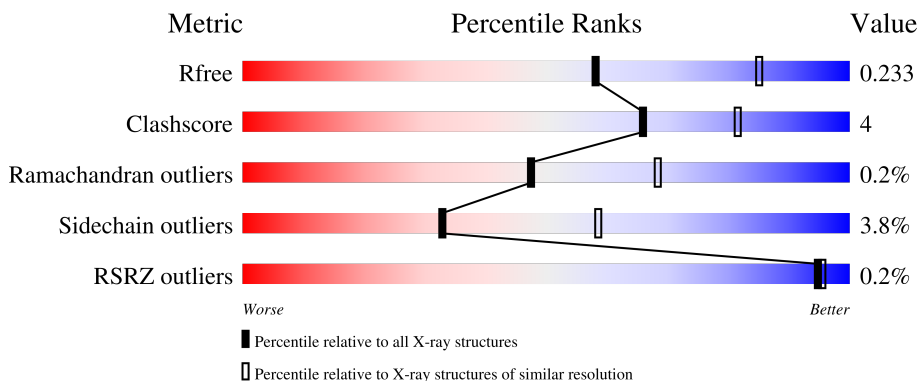
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	474	80% 10% • 9%
1	B	474	81% 9% 9%
1	C	474	80% 10% • 9%
1	D	474	81% 9% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BAL	A	600	-	X	-	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 13687 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	432	3358	2118	576	648	16	0	1	0
1	B	432	3349	2113	574	646	16	0	0	0
1	C	432	3357	2117	576	648	16	0	1	0
1	D	432	3349	2113	574	646	16	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	GLN	-	expression tag	UNP Q96W94
A	457	PHE	-	expression tag	UNP Q96W94
A	458	PRO	-	expression tag	UNP Q96W94
A	459	GLY	-	expression tag	UNP Q96W94
A	460	ASP	-	expression tag	UNP Q96W94
A	461	ASP	-	expression tag	UNP Q96W94
A	462	ASP	-	expression tag	UNP Q96W94
A	463	ASP	-	expression tag	UNP Q96W94
A	464	LYS	-	expression tag	UNP Q96W94
A	465	HIS	-	expression tag	UNP Q96W94
A	466	HIS	-	expression tag	UNP Q96W94
A	467	HIS	-	expression tag	UNP Q96W94
A	468	HIS	-	expression tag	UNP Q96W94
A	469	HIS	-	expression tag	UNP Q96W94
A	470	HIS	-	expression tag	UNP Q96W94
A	471	HIS	-	expression tag	UNP Q96W94
A	472	HIS	-	expression tag	UNP Q96W94
A	473	SER	-	expression tag	UNP Q96W94
A	474	GLY	-	expression tag	UNP Q96W94
A	475	ASP	-	expression tag	UNP Q96W94
B	456	GLN	-	expression tag	UNP Q96W94

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Chain	Residue	Modelled	Actual	Comment	Reference
B	457	PHE	-	expression tag	UNP Q96W94
B	458	PRO	-	expression tag	UNP Q96W94
B	459	GLY	-	expression tag	UNP Q96W94
B	460	ASP	-	expression tag	UNP Q96W94
B	461	ASP	-	expression tag	UNP Q96W94
B	462	ASP	-	expression tag	UNP Q96W94
B	463	ASP	-	expression tag	UNP Q96W94
B	464	LYS	-	expression tag	UNP Q96W94
B	465	HIS	-	expression tag	UNP Q96W94
B	466	HIS	-	expression tag	UNP Q96W94
B	467	HIS	-	expression tag	UNP Q96W94
B	468	HIS	-	expression tag	UNP Q96W94
B	469	HIS	-	expression tag	UNP Q96W94
B	470	HIS	-	expression tag	UNP Q96W94
B	471	HIS	-	expression tag	UNP Q96W94
B	472	HIS	-	expression tag	UNP Q96W94
B	473	SER	-	expression tag	UNP Q96W94
B	474	GLY	-	expression tag	UNP Q96W94
B	475	ASP	-	expression tag	UNP Q96W94
C	456	GLN	-	expression tag	UNP Q96W94
C	457	PHE	-	expression tag	UNP Q96W94
C	458	PRO	-	expression tag	UNP Q96W94
C	459	GLY	-	expression tag	UNP Q96W94
C	460	ASP	-	expression tag	UNP Q96W94
C	461	ASP	-	expression tag	UNP Q96W94
C	462	ASP	-	expression tag	UNP Q96W94
C	463	ASP	-	expression tag	UNP Q96W94
C	464	LYS	-	expression tag	UNP Q96W94
C	465	HIS	-	expression tag	UNP Q96W94
C	466	HIS	-	expression tag	UNP Q96W94
C	467	HIS	-	expression tag	UNP Q96W94
C	468	HIS	-	expression tag	UNP Q96W94
C	469	HIS	-	expression tag	UNP Q96W94
C	470	HIS	-	expression tag	UNP Q96W94
C	471	HIS	-	expression tag	UNP Q96W94
C	472	HIS	-	expression tag	UNP Q96W94
C	473	SER	-	expression tag	UNP Q96W94
C	474	GLY	-	expression tag	UNP Q96W94
C	475	ASP	-	expression tag	UNP Q96W94
D	456	GLN	-	expression tag	UNP Q96W94
D	457	PHE	-	expression tag	UNP Q96W94
D	458	PRO	-	expression tag	UNP Q96W94

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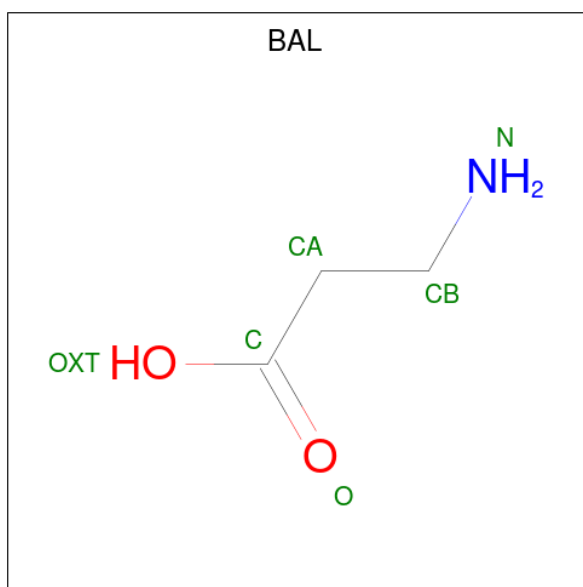
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Chain	Residue	Modelled	Actual	Comment	Reference
D	459	GLY	-	expression tag	UNP Q96W94
D	460	ASP	-	expression tag	UNP Q96W94
D	461	ASP	-	expression tag	UNP Q96W94
D	462	ASP	-	expression tag	UNP Q96W94
D	463	ASP	-	expression tag	UNP Q96W94
D	464	LYS	-	expression tag	UNP Q96W94
D	465	HIS	-	expression tag	UNP Q96W94
D	466	HIS	-	expression tag	UNP Q96W94
D	467	HIS	-	expression tag	UNP Q96W94
D	468	HIS	-	expression tag	UNP Q96W94
D	469	HIS	-	expression tag	UNP Q96W94
D	470	HIS	-	expression tag	UNP Q96W94
D	471	HIS	-	expression tag	UNP Q96W94
D	472	HIS	-	expression tag	UNP Q96W94
D	473	SER	-	expression tag	UNP Q96W94
D	474	GLY	-	expression tag	UNP Q96W94
D	475	ASP	-	expression tag	UNP Q96W94

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

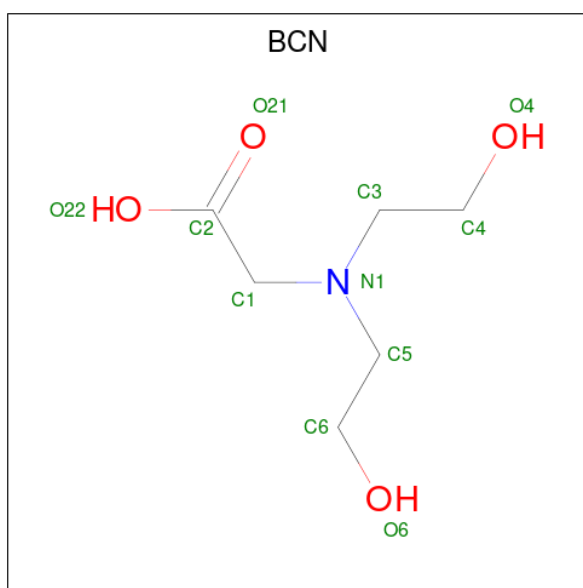
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0

- Molecule 3 is BETA-ALANINE (three-letter code: BAL) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	6	3	1	2	0	0
3	D	1	6	3	1	2	0	0

- Molecule 4 is BICINE (three-letter code: BCN) (formula:  $C_6H_{13}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	11	6	1	4	0	0
4	B	1	11	6	1	4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			11	6	1	4		
4	D	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total	O	0	0
			77	77		
5	B	45	Total	O	0	0
			45	45		
5	C	23	Total	O	0	0
			23	23		
5	D	65	Total	O	0	0
			65	65		

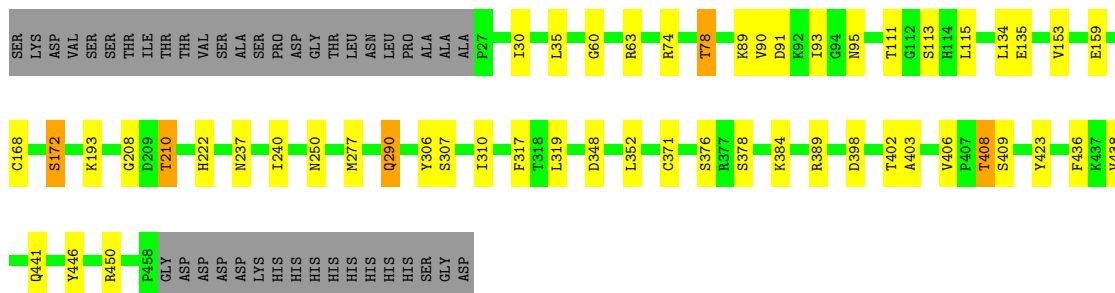


### 3 Residue-property plots [i](#)


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 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.

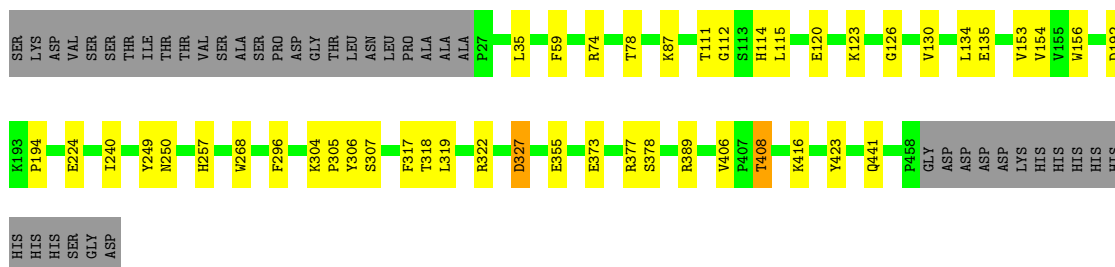
#### • Molecule 1: BETA-ALANINE SYNTHASE

Chain A: 




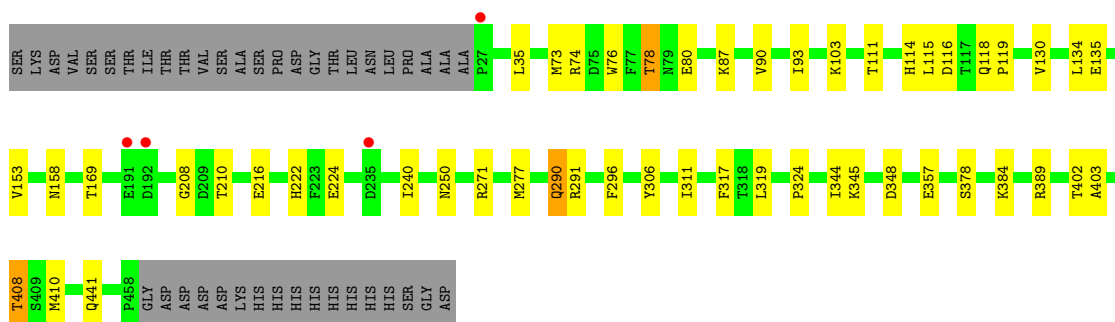
#### • Molecule 1: BETA-ALANINE SYNTHASE

Chain B: 




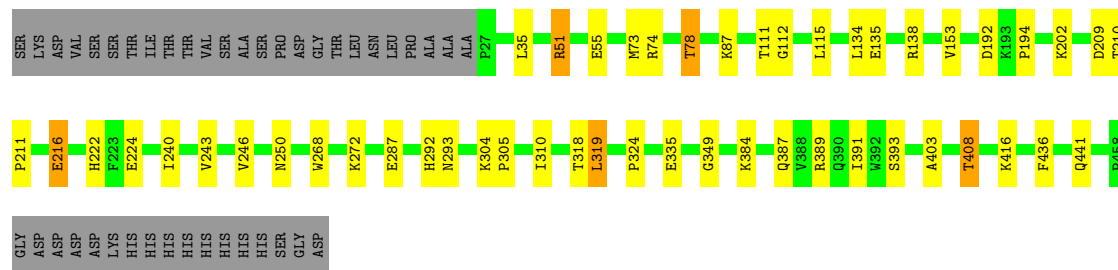
#### • Molecule 1: BETA-ALANINE SYNTHASE

Chain C: 



- Molecule 1: BETA-ALANINE SYNTHASE

Chain D:  81% 9% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.10Å 217.30Å 81.60Å 90.00° 91.90° 90.00°	Depositor
Resolution (Å)	19.84 – 2.50 19.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.84-2.50) 99.8 (19.84-2.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.94 (at 2.50Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.189 , 0.231 0.190 , 0.233	Depositor DCC
$R_{free}$ test set	2931 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtrriage
Anisotropy	0.389	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 10.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BAL, ZN, BCN

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	0.52	0/3437	0.59	0/4659
1	B	0.49	0/3428	0.55	0/4647
1	C	0.48	0/3436	0.55	0/4658
1	D	0.50	0/3428	0.58	0/4647
All	All	0.50	0/13729	0.57	0/18611

There are no bond length outliers.

There are no bond angle outliers.

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	3358	0	3236	30	0
1	B	3349	0	3229	24	0
1	C	3357	0	3234	27	0
1	D	3349	0	3229	26	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
3	A	6	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	6	0	0
4	A	11	0	12	1	0
4	B	11	0	12	1	0
4	C	11	0	12	1	0
4	D	11	0	12	2	0
5	A	77	0	0	2	0
5	B	45	0	0	1	0
5	C	23	0	0	0	0
5	D	65	0	0	1	0
All	All	13687	0	12988	107	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 4.

All (107) 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:319:LEU:N	1:D:319:LEU:CD2	2.35	0.90
1:D:318:THR:C	1:D:319:LEU:HD22	1.99	0.83
1:D:319:LEU:N	1:D:319:LEU:HD22	1.93	0.81
1:C:317:PHE:HE1	1:C:319:LEU:HD21	1.51	0.76
1:B:59:PHE:O	1:B:123:LYS:HE2	1.86	0.74
1:B:115:LEU:HD21	1:B:130:VAL:HG21	1.72	0.71
1:C:74:ARG:O	1:C:78:THR:HG22	1.92	0.70
1:A:371:CYS:HB3	1:A:409:SER:HB3	1.75	0.69
1:D:74:ARG:O	1:D:78:THR:HG22	1.93	0.68
1:A:317:PHE:HE1	1:A:319:LEU:HD21	1.60	0.66
1:B:296:PHE:HE1	1:B:319:LEU:HD22	1.60	0.66
4:B:601:BCN:H52	5:B:2045:HOH:O	1.96	0.64
1:A:317:PHE:CE1	1:A:319:LEU:HD21	2.31	0.64
1:B:317:PHE:CE1	1:B:319:LEU:HD21	2.31	0.64
1:A:63:ARG:NH1	1:A:115:LEU:O	2.30	0.64
1:B:35:LEU:HB2	1:B:135:GLU:HG3	1.79	0.63
1:B:317:PHE:HE1	1:B:319:LEU:HD21	1.62	0.63
1:D:135:GLU:OE1	1:D:138:ARG:HD2	1.98	0.63
1:B:296:PHE:CE1	1:B:319:LEU:HD22	2.34	0.63
1:D:384:LYS:H	1:D:387:GLN:HE21	1.49	0.60
1:A:403:ALA:HA	1:A:408:THR:HG23	1.82	0.60
1:A:222:HIS:HB3	1:A:408:THR:HB	1.83	0.60
1:A:406:VAL:O	1:A:408:THR:HG22	2.02	0.60
1:D:319:LEU:N	1:D:319:LEU:HD23	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:O	1:A:78:THR:HG22	2.03	0.59
1:A:371:CYS:HB3	1:A:409:SER:CB	2.33	0.59
1:B:112:GLY:O	1:B:224:GLU:HG3	2.03	0.58
1:C:93:ILE:O	1:C:93:ILE:HG13	2.03	0.58
1:D:35:LEU:HB2	1:D:135:GLU:HG3	1.84	0.58
1:D:403:ALA:HA	1:D:408:THR:HG23	1.85	0.57
1:C:403:ALA:HA	1:C:408:THR:HG23	1.87	0.57
1:C:296:PHE:CE1	1:C:319:LEU:HD22	2.40	0.57
1:C:324:PRO:HB2	4:C:601:BCN:H42	1.87	0.56
1:C:118:GLN:HB3	1:C:119:PRO:HD2	1.89	0.55
1:C:35:LEU:HB2	1:C:135:GLU:HG3	1.89	0.55
1:B:373:GLU:OE1	1:B:377:ARG:NE	2.41	0.54
1:D:292:HIS:HE1	1:D:335:GLU:OE1	1.91	0.54
1:A:35:LEU:HB2	1:A:135:GLU:HG3	1.89	0.53
1:A:74:ARG:O	1:A:78:THR:CG2	2.57	0.53
1:C:296:PHE:HE1	1:C:319:LEU:HD22	1.73	0.52
1:A:403:ALA:HA	1:A:408:THR:CG2	2.39	0.52
1:A:378:SER:OG	1:A:441:GLN:HB3	2.10	0.51
1:A:210:THR:HG22	5:A:2013:HOH:O	2.10	0.50
1:A:277:MET:HG3	1:A:352:LEU:HD22	1.93	0.50
1:C:73:MET:HG3	1:C:115:LEU:HD13	1.92	0.50
1:C:317:PHE:CE1	1:C:319:LEU:HD21	2.38	0.50
1:B:304:LYS:HB3	1:B:305:PRO:HA	1.94	0.50
1:B:74:ARG:O	1:B:78:THR:HG22	2.13	0.48
4:D:601:BCN:H62	5:D:2065:HOH:O	2.12	0.48
1:A:290:GLN:HG3	1:B:268:TRP:CE2	2.49	0.48
1:B:257:HIS:HE1	1:B:355:GLU:OE2	1.97	0.48
1:C:378:SER:OG	1:C:441:GLN:HB3	2.14	0.48
1:D:73:MET:HG3	1:D:115:LEU:HD13	1.95	0.47
1:D:112:GLY:O	1:D:224:GLU:HG3	2.14	0.47
1:D:211:PRO:HB2	1:D:216:GLU:HG3	1.96	0.47
1:A:402:THR:OG1	1:A:408:THR:HG21	2.15	0.47
1:A:307:SER:HB3	1:A:310:ILE:HG13	1.96	0.47
1:B:249:TYR:HB3	1:B:322:ARG:HD3	1.97	0.46
1:C:402:THR:OG1	1:C:408:THR:HG21	2.16	0.46
1:B:378:SER:OG	1:B:441:GLN:HB3	2.15	0.46
1:D:272:LYS:HE2	1:D:349:GLY:O	2.15	0.46
1:A:90:VAL:O	1:A:208:GLY:HA3	2.15	0.46
1:A:89:LYS:HB3	1:A:210:THR:HG21	1.98	0.46
1:A:93:ILE:HG13	1:A:93:ILE:O	2.16	0.46
1:D:135:GLU:HB3	1:D:436:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:PRO:HB2	4:D:601:BCN:H52	1.98	0.45
1:D:192:ASP:O	1:D:194:PRO:HD3	2.16	0.45
1:B:318:THR:O	1:B:319:LEU:HD23	2.15	0.45
1:C:115:LEU:HD21	1:C:130:VAL:HG21	1.98	0.45
1:C:290:GLN:HG3	1:D:268:TRP:CE2	2.52	0.45
1:C:76:TRP:CH2	1:C:80:GLU:HG3	2.52	0.45
4:A:601:BCN:H12	4:A:601:BCN:H61	1.54	0.45
1:B:154:VAL:HG11	1:B:156:TRP:CE2	2.51	0.45
1:D:304:LYS:HB3	1:D:305:PRO:HA	1.99	0.45
1:B:111:THR:O	1:B:153:VAL:HA	2.16	0.45
1:D:111:THR:O	1:D:153:VAL:HA	2.17	0.45
1:B:406:VAL:O	1:B:408:THR:HG23	2.17	0.44
1:B:327:ASP:OD1	1:B:327:ASP:N	2.51	0.44
1:B:192:ASP:O	1:B:194:PRO:HD3	2.18	0.44
1:C:222:HIS:HB3	1:C:408:THR:HB	1.99	0.44
1:B:120:GLU:HG2	1:B:423:TYR:OH	2.18	0.44
1:B:114:HIS:CE1	1:B:126:GLY:HA3	2.53	0.43
1:C:103:LYS:HE2	1:C:103:LYS:HB3	1.87	0.43
1:C:111:THR:O	1:C:153:VAL:HA	2.19	0.43
1:C:158:ASN:HB3	1:C:169:THR:HB	2.00	0.43
1:C:271:ARG:HG2	1:C:311:ILE:HD13	1.99	0.43
1:B:115:LEU:HD21	1:B:130:VAL:CG2	2.42	0.42
1:A:91:ASP:OD2	1:A:95:ASN:HB2	2.19	0.42
1:A:111:THR:O	1:A:153:VAL:HA	2.20	0.42
1:D:246:VAL:HG22	1:D:393:SER:HB3	2.01	0.42
1:C:277:MET:HE2	1:C:344:ILE:HD12	2.00	0.41
1:D:222:HIS:O	1:D:408:THR:HB	2.20	0.41
1:A:30:ILE:HG12	1:A:436:PHE:HE2	1.85	0.41
1:A:446:TYR:CE2	1:A:450:ARG:HD2	2.55	0.41
1:C:118:GLN:HB3	1:D:310:ILE:HD11	2.02	0.41
1:D:74:ARG:O	1:D:78:THR:CG2	2.66	0.41
1:A:159:GLU:HG3	1:A:398:ASP:OD2	2.20	0.41
1:A:240:ILE:HG12	1:A:438:VAL:HG21	2.01	0.41
1:D:243:VAL:HA	1:D:391:ILE:O	2.21	0.41
1:A:210:THR:CG2	5:A:2013:HOH:O	2.66	0.41
1:C:90:VAL:O	1:C:208:GLY:HA3	2.21	0.41
1:C:114:HIS:HB2	1:C:116:ASP:OD1	2.21	0.41
1:C:224:GLU:HB3	1:C:410:MET:HG2	2.02	0.41
1:A:60:GLY:HA3	1:A:423:TYR:CD2	2.56	0.40
1:D:51:ARG:NH2	1:D:55:GLU:O	2.55	0.40
1:C:115:LEU:HD21	1:C:130:VAL:CG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:CYS:O	1:A:172:SER:HB2	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	431/474 (91%)	419 (97%)	10 (2%)	2 (0%)	29	48
1	B	430/474 (91%)	416 (97%)	13 (3%)	1 (0%)	47	68
1	C	431/474 (91%)	418 (97%)	12 (3%)	1 (0%)	47	68
1	D	430/474 (91%)	416 (97%)	14 (3%)	0	100	100
All	All	1722/1896 (91%)	1669 (97%)	49 (3%)	4 (0%)	47	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	TYR
1	A	113	SER
1	B	306	TYR
1	C	306	TYR

### 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	359/393 (91%)	346 (96%)	13 (4%)	35	61
1	B	358/393 (91%)	349 (98%)	9 (2%)	47	73
1	C	359/393 (91%)	344 (96%)	15 (4%)	30	54
1	D	358/393 (91%)	341 (95%)	17 (5%)	26	49
All	All	1434/1572 (91%)	1380 (96%)	54 (4%)	33	58

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	THR
1	A	134	LEU
1	A	172	SER
1	A	193	LYS
1	A	210	THR
1	A	237	ASN
1	A	250	ASN
1	A	290	GLN
1	A	348	ASP
1	A	376	SER
1	A	384	LYS
1	A	389	ARG
1	A	408	THR
1	B	87	LYS
1	B	134	LEU
1	B	240	ILE
1	B	250	ASN
1	B	307	SER
1	B	327	ASP
1	B	389	ARG
1	B	408	THR
1	B	416	LYS
1	C	78	THR
1	C	87	LYS
1	C	134	LEU
1	C	210	THR
1	C	216	GLU
1	C	240	ILE
1	C	250	ASN
1	C	290	GLN
1	C	291	ARG
1	C	345	LYS
1	C	348	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	357	GLU
1	C	384	LYS
1	C	389	ARG
1	C	408	THR
1	D	51	ARG
1	D	78	THR
1	D	87	LYS
1	D	134	LEU
1	D	202	LYS
1	D	209	ASP
1	D	210	THR
1	D	216	GLU
1	D	240	ILE
1	D	250	ASN
1	D	287	GLU
1	D	293	ASN
1	D	319	LEU
1	D	389	ARG
1	D	408	THR
1	D	416	LYS
1	D	441	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	237	ASN
1	A	250	ASN
1	A	290	GLN
1	A	401	GLN
1	A	445	ASN
1	A	448	ASN
1	B	104	ASN
1	B	250	ASN
1	B	252	GLN
1	B	257	HIS
1	B	290	GLN
1	B	292	HIS
1	B	441	GLN
1	B	445	ASN
1	C	37	GLN
1	C	54	GLN
1	C	237	ASN

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Mol	Chain	Res	Type
1	C	250	ASN
1	C	252	GLN
1	C	290	GLN
1	C	366	ASN
1	C	441	GLN
1	C	445	ASN
1	D	79	ASN
1	D	250	ASN
1	D	257	HIS
1	D	292	HIS
1	D	387	GLN
1	D	445	ASN

### 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 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z  > 2$
4	BCN	D	601	-	10,10,10	0.68	0	11,11,11	0.71	0
4	BCN	C	601	-	10,10,10	0.72	0	11,11,11	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BCN	A	601	-	10,10,10	0.86	0	11,11,11	0.71	0
3	BAL	D	600	-	5,5,5	1.31	1 (20%)	5,5,5	1.77	2 (40%)
4	BCN	B	601	-	10,10,10	0.89	0	11,11,11	0.79	0
3	BAL	A	600	-	5,5,5	1.25	1 (20%)	5,5,5	1.89	2 (40%)

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
4	BCN	D	601	-	-	5/10/10/10	-
4	BCN	C	601	-	-	6/10/10/10	-
4	BCN	A	601	-	-	8/10/10/10	-
3	BAL	D	600	-	-	0/3/3/3	-
4	BCN	B	601	-	-	6/10/10/10	-
3	BAL	A	600	-	-	3/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	600	BAL	OXT-C	-2.42	1.22	1.30
3	A	600	BAL	OXT-C	-2.33	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	BAL	OXT-C-O	-3.05	115.70	123.30
3	D	600	BAL	OXT-C-O	-3.03	115.75	123.30
3	A	600	BAL	OXT-C-CA	2.41	121.77	114.03
3	D	600	BAL	OXT-C-CA	2.14	120.89	114.03

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	BCN	C2-C1-N1-C3
4	A	601	BCN	N1-C1-C2-O21
4	A	601	BCN	N1-C1-C2-O22
4	A	601	BCN	N1-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
4	B	601	BCN	N1-C1-C2-O21
4	B	601	BCN	N1-C1-C2-O22
4	D	601	BCN	N1-C1-C2-O21
4	A	601	BCN	C6-C5-N1-C1
4	D	601	BCN	N1-C1-C2-O22
4	D	601	BCN	C2-C1-N1-C3
4	C	601	BCN	N1-C1-C2-O21
4	A	601	BCN	N1-C5-C6-O6
4	C	601	BCN	N1-C3-C4-O4
4	B	601	BCN	C6-C5-N1-C1
4	B	601	BCN	N1-C3-C4-O4
4	C	601	BCN	N1-C1-C2-O22
4	C	601	BCN	N1-C5-C6-O6
4	D	601	BCN	N1-C3-C4-O4
4	B	601	BCN	N1-C5-C6-O6
4	B	601	BCN	C4-C3-N1-C1
3	A	600	BAL	O-C-CA-CB
3	A	600	BAL	OXT-C-CA-CB
3	A	600	BAL	C-CA-CB-N
4	D	601	BCN	N1-C5-C6-O6
4	C	601	BCN	C4-C3-N1-C5
4	A	601	BCN	C2-C1-N1-C5
4	A	601	BCN	C6-C5-N1-C3
4	C	601	BCN	C4-C3-N1-C1

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	601	BCN	2	0
4	C	601	BCN	1	0
4	A	601	BCN	1	0
4	B	601	BCN	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	432/474 (91%)	-0.64	0 100 100	22, 26, 30, 36	0
1	B	432/474 (91%)	-0.52	0 100 100	22, 26, 29, 35	0
1	C	432/474 (91%)	-0.50	4 (0%) 84 86	22, 26, 29, 36	0
1	D	432/474 (91%)	-0.64	0 100 100	22, 26, 30, 36	0
All	All	1728/1896 (91%)	-0.58	4 (0%) 95 95	22, 26, 30, 36	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	ASP	4.3
1	C	235	ASP	2.4
1	C	27	PRO	2.4
1	C	191	GLU	2.1

### 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 monosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	BCN	C	601	11/11	0.83	0.14	43,44,45,45	0
4	BCN	A	601	11/11	0.88	0.14	45,47,48,48	0
4	BCN	D	601	11/11	0.90	0.12	47,47,49,49	0
4	BCN	B	601	11/11	0.91	0.14	40,42,45,45	0
3	BAL	A	600	6/6	0.95	0.12	40,41,41,41	0
3	BAL	D	600	6/6	0.95	0.14	37,37,38,38	0
2	ZN	C	500	1/1	0.98	0.07	36,36,36,36	0
2	ZN	C	501	1/1	0.98	0.03	53,53,53,53	0
2	ZN	A	501	1/1	0.98	0.05	54,54,54,54	0
2	ZN	B	501	1/1	0.98	0.04	58,58,58,58	0
2	ZN	D	500	1/1	0.99	0.10	42,42,42,42	0
2	ZN	D	501	1/1	0.99	0.04	62,62,62,62	0
2	ZN	B	500	1/1	1.00	0.11	38,38,38,38	0
2	ZN	A	500	1/1	1.00	0.07	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.