Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:53 AM GMT

PDB ID	:	2V8D
Title	:	CRYSTAL STRUCTURE OF MUTANT E159A OF BETA-ALANINE SYNTHASE FROM SACCHAROMYCES KLUYVERI
Authors	:	Lundgren, S.; Andersen, B.; Piskur, J.; Dobritzsch, D.
Deposited on	:	2007-08-07
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

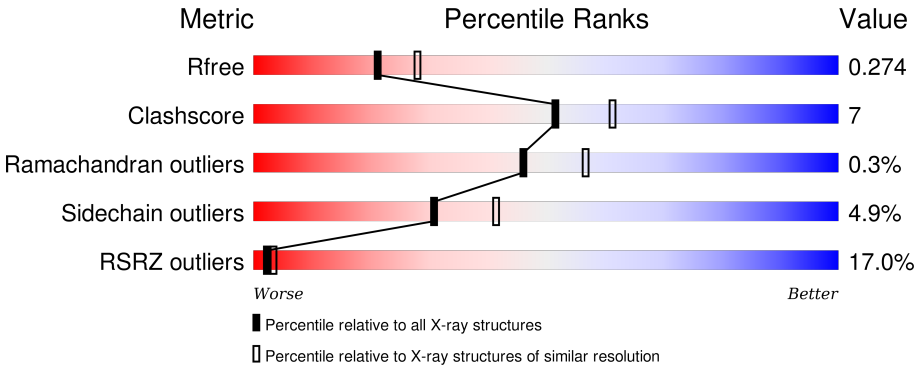
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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% 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	8% 77% 15% • 8%
1	B	474	23% 74% 15% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6747 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	437	Total	C	N	O	S	0	1	0
			3371	2126	578	651	16			
1	B	429	Total	C	N	O	S	0	0	0
			3314	2090	568	640	16			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	ALA	GLU	ENGINEERED MUTATION	UNP Q96W94
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	159	ALA	GLU	ENGINEERED MUTATION	UNP Q96W94
B	456	GLN	-	EXPRESSION TAG	UNP Q96W94
B	457	PHE	-	EXPRESSION TAG	UNP Q96W94
B	458	PRO	-	EXPRESSION TAG	UNP Q96W94

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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 water.

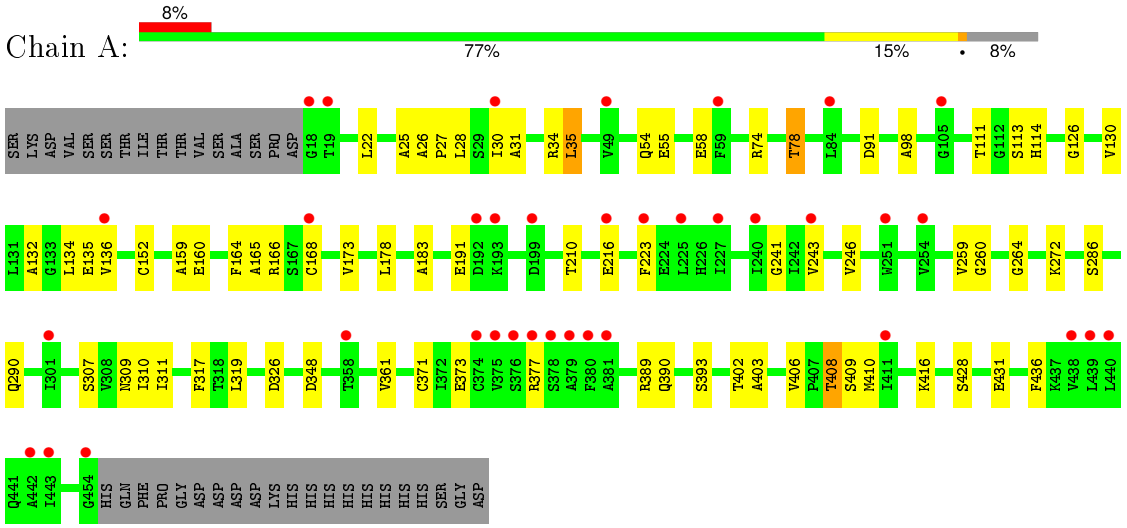
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	42	Total O 42 42	0	0
3	B	16	Total O 16 16	0	0

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 errors 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.

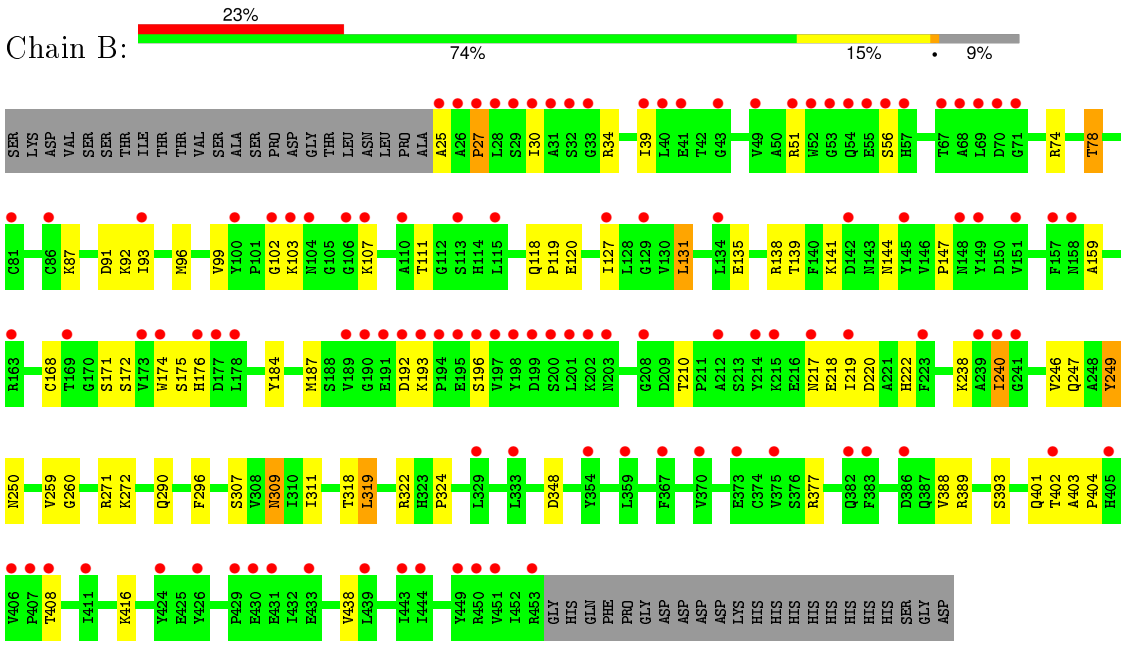
- Molecule 1: BETA-ALANINE SYNTHASE

Chain A:



- Molecule 1: BETA-ALANINE SYNTHASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.12Å 77.14Å 108.23Å 90.00° 97.12° 90.00°	Depositor
Resolution (Å)	45.22 – 2.30 45.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (45.22-2.30) 96.6 (45.24-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.276 0.230 , 0.274	Depositor DCC
R_{free} test set	2195 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 43034 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6747	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.50	0/3451	0.60	0/4681
1	B	0.41	0/3390	0.52	0/4597
All	All	0.45	0/6841	0.56	0/9278

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

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	3371	0	3264	42	0
1	B	3314	0	3203	49	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	42	0	0	0	0
3	B	16	0	0	0	0
All	All	6747	0	6467	89	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 7.

All (89) 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:25:ALA:O	1:A:27:PRO:HD3	1.39	1.20
1:A:74:ARG:O	1:A:78:THR:HG22	1.62	1.00
1:B:25:ALA:O	1:B:27:PRO:HD3	1.65	0.96
1:B:107:LYS:HE2	1:B:218:GLU:HB2	1.56	0.87
1:B:238:LYS:HG2	1:B:389:ARG:HG2	1.65	0.78
1:B:296:PHE:HE1	1:B:319:LEU:HD12	1.53	0.74
1:B:168:CYS:O	1:B:172:SER:HB2	1.90	0.71
1:A:160:GLU:OE1	1:A:160:GLU:HA	1.88	0.71
1:A:74:ARG:O	1:A:78:THR:CG2	2.40	0.69
1:A:178:LEU:HD21	1:A:183:ALA:HB2	1.75	0.68
1:B:318:THR:C	1:B:319:LEU:HD22	2.14	0.68
1:B:319:LEU:HD22	1:B:319:LEU:N	2.09	0.67
1:B:296:PHE:CE1	1:B:319:LEU:HD12	2.29	0.67
1:B:296:PHE:HE1	1:B:319:LEU:CD1	2.09	0.65
1:A:55:GLU:HB2	1:A:58:GLU:CD	2.19	0.64
1:B:51:ARG:HH22	1:B:56:SER:HA	1.65	0.61
1:B:247:GLN:HE21	1:B:324:PRO:HD3	1.67	0.58
1:A:246:VAL:HG22	1:A:393:SER:HB3	1.85	0.58
1:B:102:GLY:HA2	1:B:147:PRO:HG2	1.86	0.58
1:A:406:VAL:HG23	1:A:408:THR:HG22	1.85	0.58
1:A:286:SER:O	1:A:290:GLN:HG3	2.05	0.57
1:A:309:ASN:OD1	1:B:322:ARG:NH2	2.39	0.56
1:A:25:ALA:O	1:A:27:PRO:CD	2.33	0.55
1:A:35:LEU:O	1:A:35:LEU:HD12	2.07	0.55
1:B:175:SER:O	1:B:176:HIS:HB2	2.07	0.54
1:B:78:THR:HG22	1:B:96:MET:CE	2.38	0.54
1:A:34:ARG:NE	1:A:135:GLU:OE1	2.40	0.54
1:B:127:ILE:HG22	1:B:131:LEU:HD22	1.91	0.53
1:A:22:LEU:HD12	1:A:377:ARG:HD3	1.91	0.53
1:B:39:ILE:HG12	1:B:131:LEU:HD23	1.91	0.53
1:B:319:LEU:N	1:B:319:LEU:CD2	2.72	0.52
1:A:132:ALA:O	1:A:136:VAL:HG23	2.10	0.52
1:B:307:SER:C	1:B:309:ASN:H	2.11	0.52
1:A:389:ARG:HD3	1:A:390:GLN:O	2.09	0.52
1:A:178:LEU:CD2	1:A:183:ALA:HB2	2.37	0.52
1:A:428:SER:OG	1:A:431:GLU:HG3	2.10	0.52
1:B:271:ARG:CZ	1:B:311:ILE:HD11	2.40	0.52
1:B:296:PHE:CE1	1:B:319:LEU:CD1	2.91	0.51
1:A:30:ILE:HG22	1:A:31:ALA:N	2.25	0.50
1:A:259:VAL:HG23	1:A:272:LYS:HD2	1.94	0.50
1:A:114:HIS:CE1	1:A:126:GLY:HA3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:VAL:HG23	1:B:272:LYS:HD2	1.93	0.49
1:B:78:THR:HG22	1:B:96:MET:HE3	1.94	0.49
1:B:91:ASP:HA	1:B:210:THR:HB	1.94	0.49
1:B:240:ILE:HG22	1:B:388:VAL:HG13	1.94	0.49
1:B:174:TRP:HE1	1:B:217:ASN:HB3	1.77	0.48
1:B:246:VAL:HG22	1:B:393:SER:HB3	1.95	0.48
1:B:403:ALA:N	1:B:404:PRO:HD2	2.29	0.48
1:A:260:GLY:HA2	1:A:311:ILE:O	2.14	0.48
1:A:317:PHE:CE1	1:A:319:LEU:HD21	2.48	0.48
1:A:98:ALA:O	1:A:152:CYS:HA	2.14	0.47
1:B:171:SER:HB2	1:B:401:GLN:HB2	1.96	0.47
1:A:402:THR:OG1	1:A:408:THR:HG21	2.15	0.47
1:B:222:HIS:HB3	1:B:408:THR:HG22	1.97	0.47
1:B:34:ARG:NH2	1:B:138:ARG:HB3	2.29	0.47
1:A:35:LEU:C	1:A:35:LEU:HD12	2.34	0.47
1:B:30:ILE:HG22	1:B:139:THR:HG21	1.97	0.46
1:A:91:ASP:HA	1:A:210:THR:O	2.15	0.46
1:A:111:THR:HA	1:A:223:PHE:O	2.17	0.45
1:A:35:LEU:HD23	1:A:436:PHE:HB2	1.97	0.45
1:A:173:VAL:HG23	1:A:178:LEU:HD23	1.99	0.45
1:B:184:TYR:O	1:B:196:SER:HB2	2.16	0.45
1:B:74:ARG:O	1:B:78:THR:HG23	2.17	0.45
1:B:159:ALA:HA	1:B:168:CYS:HA	1.99	0.44
1:B:249:TYR:CD1	1:B:249:TYR:C	2.91	0.44
1:B:260:GLY:HA2	1:B:311:ILE:O	2.17	0.44
1:A:173:VAL:HA	1:A:178:LEU:O	2.18	0.44
1:B:402:THR:OG1	1:B:408:THR:HG21	2.17	0.44
1:A:113:SER:HB3	1:A:126:GLY:O	2.18	0.44
1:A:371:CYS:HB3	1:A:409:SER:HB2	2.01	0.43
1:A:159:ALA:HA	1:A:168:CYS:H	1.84	0.43
1:B:403:ALA:N	1:B:404:PRO:CD	2.82	0.43
1:B:118:GLN:HB3	1:B:119:PRO:CD	2.49	0.42
1:A:264:GLY:HA2	1:B:322:ARG:HD2	2.00	0.42
1:B:87:LYS:O	1:B:99:VAL:N	2.53	0.42
1:B:107:LYS:CE	1:B:218:GLU:HB2	2.39	0.42
1:B:107:LYS:HE3	1:B:218:GLU:O	2.20	0.42
1:A:241:GLY:HA2	1:A:389:ARG:O	2.19	0.42
1:A:403:ALA:HA	1:A:408:THR:HG23	2.02	0.41
1:A:307:SER:C	1:A:309:ASN:H	2.23	0.41
1:B:118:GLN:HB3	1:B:119:PRO:HD2	2.02	0.41
1:B:103:LYS:HB2	1:B:147:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:O	1:A:408:THR:HG23	2.20	0.41
1:B:307:SER:C	1:B:309:ASN:N	2.74	0.41
1:A:164:PHE:O	1:A:166:ARG:N	2.40	0.41
1:A:243:VAL:HB	1:A:410:MET:HB2	2.03	0.40
1:A:307:SER:HB2	1:A:310:ILE:HD12	2.02	0.40
1:B:240:ILE:HG12	1:B:438:VAL:HG21	2.02	0.40
1:B:219:ILE:HG22	1:B:220:ASP:N	2.36	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	436/474 (92%)	419 (96%)	15 (3%)	2 (0%)	34	41
1	B	427/474 (90%)	407 (95%)	19 (4%)	1 (0%)	52	64
All	All	863/948 (91%)	826 (96%)	34 (4%)	3 (0%)	46	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ALA
1	A	26	ALA
1	B	27	PRO

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	359/392 (92%)	345 (96%)	14 (4%)	39 53
1	B	353/392 (90%)	332 (94%)	21 (6%)	24 32
All	All	712/784 (91%)	677 (95%)	35 (5%)	31 41

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	35	LEU
1	A	54	GLN
1	A	78	THR
1	A	130	VAL
1	A	134	LEU
1	A	191	GLU
1	A	216	GLU
1	A	326	ASP
1	A	348	ASP
1	A	361	VAL
1	A	373	GLU
1	A	408	THR
1	A	416	LYS
1	B	78	THR
1	B	92	LYS
1	B	93	ILE
1	B	111	THR
1	B	120	GLU
1	B	131	LEU
1	B	135	GLU
1	B	141	LYS
1	B	144	ASN
1	B	187	MET
1	B	192	ASP
1	B	193	LYS
1	B	240	ILE
1	B	249	TYR
1	B	250	ASN
1	B	290	GLN
1	B	309	ASN
1	B	319	LEU
1	B	348	ASP
1	B	377	ARG

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Mol	Chain	Res	Type
1	B	416	LYS

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

Mol	Chain	Res	Type
1	A	37	GLN
1	A	79	ASN
1	A	158	ASN
1	A	203	ASN
1	A	247	GLN
1	A	360	GLN
1	A	401	GLN
1	B	247	GLN
1	B	250	ASN
1	B	309	ASN
1	B	434	ASN
1	B	441	GLN
1	B	445	ASN

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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	437/474 (92%)	0.77	37 (8%) 13 19	16, 24, 34, 45	0
1	B	429/474 (90%)	1.42	110 (25%) 1 1	20, 31, 38, 48	0
All	All	866/948 (91%)	1.09	147 (16%) 2 3	16, 26, 37, 48	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	TYR	8.2
1	B	68	ALA	7.4
1	B	444	ILE	7.3
1	B	212	ALA	7.1
1	B	239	ALA	7.1
1	B	198	TYR	6.3
1	B	189	VAL	6.3
1	B	197	VAL	6.1
1	B	93	ILE	6.0
1	B	214	TYR	5.9
1	B	375	VAL	5.8
1	B	190	GLY	5.6
1	B	67	THR	5.5
1	B	178	LEU	5.4
1	B	54	GLN	5.3
1	B	70	ASP	5.1
1	B	383	PHE	5.0
1	B	405	HIS	5.0
1	B	208	GLY	5.0
1	B	215	LYS	4.9
1	B	106	GLY	4.6
1	B	151	VAL	4.6
1	B	32	SER	4.5
1	B	158	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	191	GLU	4.4
1	B	26	ALA	4.3
1	B	426	TYR	4.3
1	B	451	VAL	4.3
1	A	192	ASP	4.2
1	B	406	VAL	4.1
1	B	192	ASP	4.1
1	B	71	GLY	4.0
1	B	223	PHE	4.0
1	B	53	GLY	3.9
1	B	52	TRP	3.9
1	B	193	LYS	3.9
1	A	18	GLY	3.9
1	B	163	ARG	3.8
1	B	199	ASP	3.8
1	B	219	ILE	3.8
1	B	104	ASN	3.8
1	B	386	ASP	3.7
1	B	55	GLU	3.6
1	B	194	PRO	3.6
1	B	196	SER	3.6
1	B	443	ILE	3.6
1	A	381	ALA	3.6
1	B	69	LEU	3.6
1	A	19	THR	3.5
1	B	102	GLY	3.5
1	B	56	SER	3.4
1	B	115	LEU	3.3
1	B	127	ILE	3.3
1	B	113	SER	3.3
1	B	429	PRO	3.3
1	B	411	ILE	3.3
1	B	169	THR	3.3
1	B	57	HIS	3.3
1	B	103	LYS	3.2
1	B	177	ASP	3.2
1	B	173	VAL	3.2
1	A	105	GLY	3.2
1	B	195	GLU	3.2
1	A	49	VAL	3.1
1	A	438	VAL	3.1
1	B	241	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	29	SER	3.0
1	B	176	HIS	3.0
1	B	370	VAL	3.0
1	B	100	TYR	3.0
1	B	453	ARG	3.0
1	B	51	ARG	2.9
1	B	430	GLU	2.9
1	A	443	ILE	2.9
1	A	377	ARG	2.9
1	B	407	PRO	2.8
1	B	145	TYR	2.8
1	B	382	GLN	2.8
1	A	378	SER	2.8
1	B	30	ILE	2.8
1	B	203	ASN	2.7
1	A	375	VAL	2.7
1	A	440	LEU	2.7
1	B	174	TRP	2.7
1	A	240	ILE	2.7
1	B	408	THR	2.6
1	B	81	CYS	2.6
1	B	431	GLU	2.6
1	A	84	LEU	2.6
1	A	411	ILE	2.6
1	B	367	PHE	2.6
1	B	449	TYR	2.6
1	A	454	GLY	2.6
1	B	129	GLY	2.5
1	B	157	PHE	2.5
1	B	424	TYR	2.5
1	B	202	LYS	2.5
1	A	199	ASP	2.5
1	B	110	ALA	2.5
1	B	107	LYS	2.4
1	B	39	ILE	2.4
1	B	217	ASN	2.4
1	A	254	VAL	2.4
1	B	359	LEU	2.4
1	A	374	CYS	2.4
1	B	43	GLY	2.3
1	B	201	LEU	2.3
1	B	240	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	59	PHE	2.3
1	A	168	CYS	2.3
1	B	33	GLY	2.3
1	B	329	LEU	2.3
1	B	134	LEU	2.3
1	A	136	VAL	2.3
1	A	223	PHE	2.3
1	A	251	TRP	2.3
1	A	193	LYS	2.3
1	A	225	LEU	2.3
1	B	25	ALA	2.2
1	A	439	LEU	2.2
1	A	216	GLU	2.2
1	A	358	THR	2.2
1	A	380	PHE	2.2
1	A	376	SER	2.2
1	B	49	VAL	2.2
1	B	200	SER	2.2
1	B	402	THR	2.2
1	B	373	GLU	2.2
1	B	333	LEU	2.1
1	B	450	ARG	2.1
1	A	301	ILE	2.1
1	B	27	PRO	2.1
1	B	433	GLU	2.1
1	B	148	ASN	2.1
1	B	86	CYS	2.1
1	B	40	LEU	2.1
1	A	379	ALA	2.1
1	B	31	ALA	2.1
1	B	354	TYR	2.1
1	B	439	LEU	2.1
1	A	30	ILE	2.0
1	A	227	ILE	2.0
1	A	243	VAL	2.0
1	B	142	ASP	2.0
1	A	442	ALA	2.0
1	B	41	GLU	2.0
1	B	28	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	B	500	1/1	0.93	0.19	0.15	48,48,48,48	0
2	ZN	A	501	1/1	0.98	0.15	-0.38	12,12,12,12	1
2	ZN	B	501	1/1	0.94	0.10	-1.92	33,33,33,33	1
2	ZN	A	500	1/1	0.97	0.14	-2.31	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.