Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 09:28 PM EDT

PDB ID	:	2CY8
Title	:	Crystal structure of D-phenylglycine aminotransferase (D-PhgAT) from Pseudomonas strutzeri ST-201
Authors	:	Kongsaeree, P.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-07-05
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
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 (1)) were used in the production of this report:

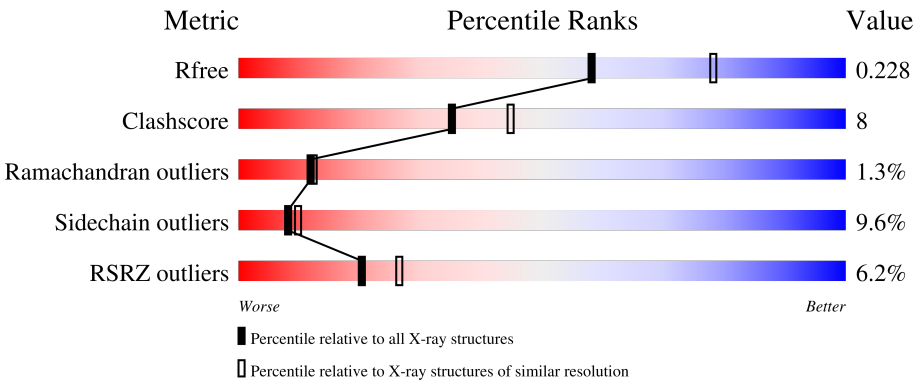
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

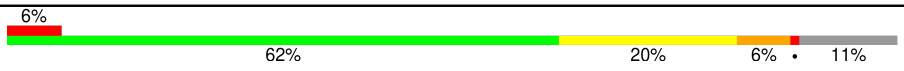
The reported resolution of this entry is 2.30 Å.

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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% 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	453	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3185 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 D-phenylglycine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3055	1926	555	562	12	0	0	0

- Molecule 2 is water.

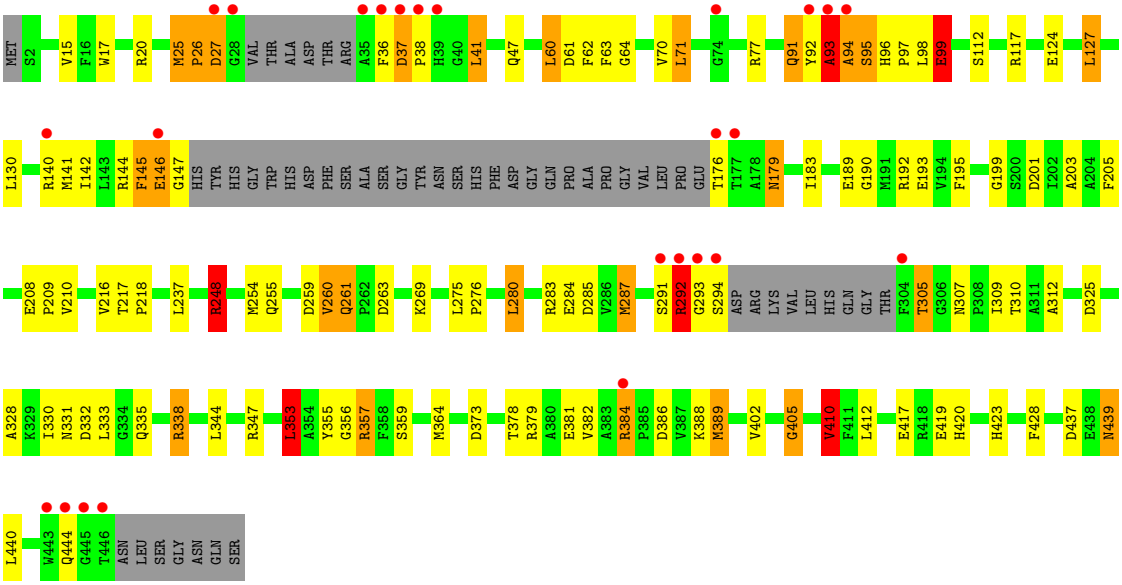
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	130	130	130	0	0

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 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: D-phenylglycine aminotransferase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	74.68Å 74.68Å 147.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.60 – 2.30 31.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (31.60-2.30) 95.4 (31.59-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.27 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.184 , 0.223 0.191 , 0.228	Depositor DCC
R_{free} test set	1073 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3185	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.74	40/3116 (1.3%)	1.40	40/4216 (0.9%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	PHE	CB-CG	-11.51	1.31	1.51
1	A	410	VAL	CB-CG2	-10.30	1.31	1.52
1	A	92	TYR	CD2-CE2	9.76	1.53	1.39
1	A	208	GLU	CD-OE1	9.04	1.35	1.25
1	A	402	VAL	CB-CG1	-8.95	1.34	1.52
1	A	189	GLU	CD-OE2	8.19	1.34	1.25
1	A	124	GLU	CD-OE2	-7.88	1.17	1.25
1	A	193	GLU	CD-OE2	7.60	1.34	1.25
1	A	439	ASN	CB-CG	-7.42	1.33	1.51
1	A	146	GLU	CB-CG	7.05	1.65	1.52
1	A	70	VAL	CB-CG1	-6.88	1.38	1.52
1	A	94	ALA	CA-CB	6.72	1.66	1.52
1	A	210	VAL	CB-CG1	-6.66	1.38	1.52
1	A	17	TRP	CB-CG	-6.14	1.39	1.50
1	A	269	LYS	CE-NZ	-6.09	1.33	1.49
1	A	124	GLU	CD-OE1	-6.02	1.19	1.25
1	A	328	ALA	CA-CB	5.94	1.65	1.52
1	A	419	GLU	CD-OE2	5.93	1.32	1.25
1	A	92	TYR	CE1-CZ	5.88	1.46	1.38
1	A	216	VAL	CB-CG2	5.85	1.65	1.52
1	A	92	TYR	CD1-CE1	5.67	1.47	1.39
1	A	146	GLU	CG-CD	5.64	1.60	1.51
1	A	260	VAL	CB-CG1	-5.51	1.41	1.52
1	A	353	LEU	CG-CD1	-5.46	1.31	1.51
1	A	189	GLU	CD-OE1	5.45	1.31	1.25
1	A	208	GLU	CD-OE2	5.43	1.31	1.25
1	A	382	VAL	CB-CG1	5.39	1.64	1.52
1	A	261	GLN	CG-CD	5.37	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	GLY	CA-C	5.33	1.60	1.51
1	A	364	MET	CB-CG	5.32	1.68	1.51
1	A	388	LYS	CD-CE	5.31	1.64	1.51
1	A	208	GLU	CG-CD	5.22	1.59	1.51
1	A	190	GLY	CA-C	5.13	1.60	1.51
1	A	312	ALA	CA-CB	-5.13	1.41	1.52
1	A	15	VAL	CB-CG2	5.12	1.63	1.52
1	A	47	GLN	CG-CD	5.09	1.62	1.51
1	A	248	ARG	CG-CD	-5.06	1.39	1.51
1	A	92	TYR	CE2-CZ	5.03	1.45	1.38
1	A	405	GLY	C-O	5.03	1.31	1.23
1	A	203	ALA	CA-CB	5.03	1.63	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	325	ASP	CB-CG-OD2	11.08	128.27	118.30
1	A	20	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	A	386	ASP	CB-CG-OD2	9.03	126.42	118.30
1	A	389	MET	CG-SD-CE	-8.72	86.25	100.20
1	A	127	LEU	CB-CG-CD1	8.38	125.24	111.00
1	A	145	PHE	CB-CA-C	-8.35	93.69	110.40
1	A	20	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	A	437	ASP	CB-CG-OD2	7.75	125.27	118.30
1	A	37	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	373	ASP	CB-CG-OD2	7.43	124.99	118.30
1	A	353	LEU	CB-CG-CD2	7.38	123.55	111.00
1	A	285	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	357	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	A	192	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	25	MET	CG-SD-CE	-6.90	89.16	100.20
1	A	183	ILE	CG1-CB-CG2	-6.55	96.99	111.40
1	A	332	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	292	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	412	LEU	CA-CB-CG	6.08	129.29	115.30
1	A	384	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	A	263	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	71	LEU	CB-CG-CD1	5.82	120.90	111.00
1	A	144	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	92	TYR	C-N-CA	5.75	136.09	121.70
1	A	99	GLU	CG-CD-OE2	5.73	129.77	118.30
1	A	217	THR	CA-CB-CG2	-5.71	104.41	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	LEU	CB-CG-CD1	-5.70	101.31	111.00
1	A	201	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	280	LEU	CB-CG-CD2	5.67	120.64	111.00
1	A	347	ARG	CA-CB-CG	5.65	125.83	113.40
1	A	259	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	61	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	248	ARG	CG-CD-NE	5.49	123.33	111.80
1	A	248	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	353	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	292	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	93	ALA	N-CA-C	5.12	124.81	111.00
1	A	95	SER	N-CA-C	-5.08	97.27	111.00
1	A	41	LEU	CB-CG-CD1	5.06	119.60	111.00
1	A	410	VAL	CA-CB-CG1	5.01	118.42	110.90

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	3055	0	3013	50	0
2	A	130	0	0	4	0
All	All	3185	0	3013	50	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 8.

All (50) 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:389:MET:SD	1:A:389:MET:CE	2.02	1.47
1:A:389:MET:CE	1:A:389:MET:CG	2.59	0.81
1:A:145:PHE:CD2	1:A:145:PHE:N	2.48	0.76
1:A:94:ALA:O	1:A:95:SER:OG	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ARG:HD2	1:A:381:GLU:OE1	1.90	0.71
1:A:275:LEU:HB3	1:A:276:PRO:HD2	1.74	0.69
1:A:112:SER:HB2	1:A:261:GLN:OE1	1.92	0.69
1:A:96:HIS:HD2	1:A:98:LEU:H	1.42	0.67
1:A:335:GLN:NE2	1:A:338:ARG:HH21	1.96	0.64
1:A:145:PHE:N	1:A:145:PHE:HD2	1.94	0.60
1:A:353:LEU:CD1	1:A:355:TYR:HB3	2.32	0.59
1:A:112:SER:HB3	1:A:255:GLN:OE1	2.03	0.58
1:A:248:ARG:HD3	1:A:359:SER:OG	2.04	0.57
1:A:356:GLY:HA2	2:A:553:HOH:O	2.04	0.57
1:A:389:MET:CE	1:A:389:MET:HG3	2.36	0.56
1:A:292:ARG:HH11	1:A:292:ARG:HG3	1.70	0.56
1:A:99:GLU:OE1	1:A:305:THR:HG22	2.07	0.55
1:A:331:ASN:ND2	2:A:494:HOH:O	2.41	0.54
1:A:417:GLU:H	1:A:420:HIS:HD2	1.54	0.53
1:A:62:PHE:HB3	1:A:410:VAL:HB	1.90	0.52
1:A:293:GLY:O	1:A:294:SER:OG	2.23	0.52
1:A:291:SER:C	1:A:292:ARG:HD3	2.30	0.52
1:A:195:PHE:O	1:A:199:GLY:HA3	2.09	0.51
1:A:25:MET:O	1:A:26:PRO:C	2.49	0.49
1:A:146:GLU:OE2	1:A:147:GLY:HA3	2.12	0.49
1:A:96:HIS:CD2	1:A:98:LEU:H	2.26	0.47
1:A:218:PRO:O	1:A:378:THR:HG22	2.16	0.46
1:A:209:PRO:HB2	1:A:254:MET:HG2	1.99	0.45
1:A:60:LEU:HD13	1:A:62:PHE:CE2	2.51	0.45
1:A:260:VAL:HG12	1:A:261:GLN:N	2.32	0.45
1:A:275:LEU:HB3	1:A:276:PRO:CD	2.46	0.45
1:A:378:THR:CG2	2:A:521:HOH:O	2.65	0.45
1:A:145:PHE:HE2	1:A:205:PHE:CZ	2.36	0.43
1:A:389:MET:HG3	1:A:440:LEU:O	2.19	0.43
1:A:293:GLY:O	1:A:294:SER:CB	2.66	0.43
1:A:141:MET:HE2	1:A:179:ASN:ND2	2.33	0.43
1:A:353:LEU:HD11	1:A:355:TYR:HB3	2.00	0.42
1:A:91:GLN:O	1:A:307:ASN:ND2	2.53	0.42
1:A:275:LEU:HD12	1:A:310:THR:HA	2.01	0.42
1:A:63:PHE:CD1	1:A:405:GLY:HA3	2.55	0.42
1:A:333:LEU:HD23	1:A:333:LEU:HA	1.83	0.41
1:A:93:ALA:HB1	1:A:96:HIS:HB2	2.02	0.41
1:A:117:ARG:NH2	1:A:291:SER:OG	2.47	0.41
1:A:330:ILE:HD13	1:A:330:ILE:HG21	1.90	0.41
1:A:60:LEU:HD12	1:A:423:HIS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HD2	2:A:580:HOH:O	2.21	0.40
1:A:335:GLN:HE21	1:A:338:ARG:HH21	1.69	0.40
1:A:283:ARG:O	1:A:287:MET:HB2	2.21	0.40
1:A:417:GLU:H	1:A:420:HIS:CD2	2.35	0.40
1:A:141:MET:CE	1:A:179:ASN:ND2	2.84	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	394/453 (87%)	370 (94%)	19 (5%)	5 (1%)	12 12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	ALA
1	A	444	GLN
1	A	27	ASP
1	A	26	PRO
1	A	38	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	311/353 (88%)	281 (90%)	30 (10%)	8 10

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	36	PHE
1	A	37	ASP
1	A	41	LEU
1	A	60	LEU
1	A	71	LEU
1	A	77	ARG
1	A	91	GLN
1	A	97	PRO
1	A	99	GLU
1	A	127	LEU
1	A	130	LEU
1	A	142	ILE
1	A	176	THR
1	A	179	ASN
1	A	248	ARG
1	A	280	LEU
1	A	284	GLU
1	A	287	MET
1	A	292	ARG
1	A	305	THR
1	A	309	ILE
1	A	338	ARG
1	A	344	LEU
1	A	353	LEU
1	A	357	ARG
1	A	384	ARG
1	A	410	VAL
1	A	428	PHE
1	A	439	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	79	ASN
1	A	91	GLN

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Mol	Chain	Res	Type
1	A	96	HIS
1	A	179	ASN
1	A	331	ASN
1	A	335	GLN
1	A	420	HIS
1	A	423	HIS

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)

There are no ligands in this entry.

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, 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	402/453 (88%)	0.02	25 (6%) 20 26	23, 36, 73, 98	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	GLY	12.3
1	A	291	SER	10.9
1	A	293	GLY	9.6
1	A	94	ALA	8.7
1	A	28	GLY	8.5
1	A	446	THR	8.3
1	A	35	ALA	7.6
1	A	177	THR	5.7
1	A	176	THR	4.9
1	A	37	ASP	4.9
1	A	444	GLN	4.4
1	A	294	SER	4.4
1	A	93	ALA	4.2
1	A	304	PHE	4.2
1	A	38	PRO	4.2
1	A	292	ARG	4.0
1	A	36	PHE	4.0
1	A	27	ASP	2.5
1	A	92	TYR	2.5
1	A	146	GLU	2.4
1	A	384	ARG	2.2
1	A	39	HIS	2.1
1	A	443	TRP	2.1
1	A	140	ARG	2.0
1	A	74	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.