



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:06 PM UTC

PDB ID : 4BIA / pdb_00004bia
Title : Crystal structure of SCP2 thiolase from Trypanosoma brucei: The C337A mutant.
Authors : Harijan, R.K.; Kiema, T.-R.; Weiss, M.S.; Michels, P.A.M.; Wierenga, R.K.
Deposited on : 2013-04-10
Resolution : 2.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

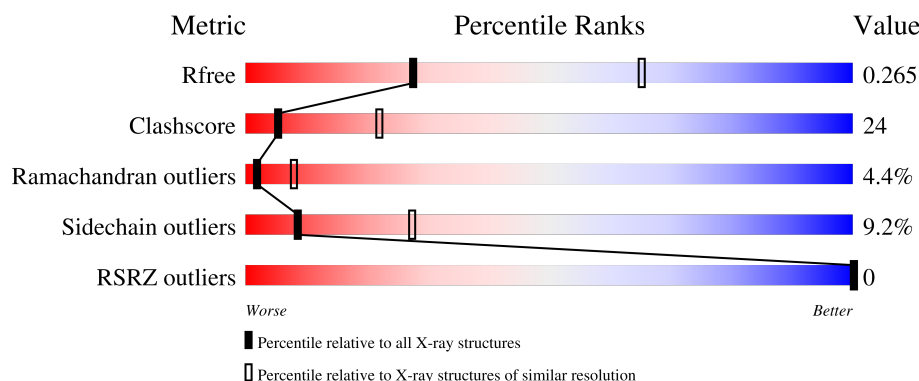
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	454	
1	B	454	
1	C	454	
1	D	454	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12319 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 3-KETOACYL-COA THIOLASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3072	1924	540	592	16			
1	B	416	Total	C	N	O	S	0	0	0
			3068	1921	542	589	16			
1	C	419	Total	C	N	O	S	0	0	0
			3086	1931	545	594	16			
1	D	416	Total	C	N	O	S	0	0	0
			3065	1920	541	588	16			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP Q57XD5
A	-14	HIS	-	expression tag	UNP Q57XD5
A	-13	HIS	-	expression tag	UNP Q57XD5
A	-12	HIS	-	expression tag	UNP Q57XD5
A	-11	HIS	-	expression tag	UNP Q57XD5
A	-10	HIS	-	expression tag	UNP Q57XD5
A	-9	SER	-	expression tag	UNP Q57XD5
A	-8	SER	-	expression tag	UNP Q57XD5
A	-7	GLY	-	expression tag	UNP Q57XD5
A	-6	LEU	-	expression tag	UNP Q57XD5
A	-5	VAL	-	expression tag	UNP Q57XD5
A	-4	PRO	-	expression tag	UNP Q57XD5
A	-3	ARG	-	expression tag	UNP Q57XD5
A	-2	GLY	-	expression tag	UNP Q57XD5
A	-1	SER	-	expression tag	UNP Q57XD5
A	0	HIS	-	expression tag	UNP Q57XD5
A	337	ALA	CYS	engineered mutation	UNP Q57XD5
B	-15	HIS	-	expression tag	UNP Q57XD5
B	-14	HIS	-	expression tag	UNP Q57XD5
B	-13	HIS	-	expression tag	UNP Q57XD5
B	-12	HIS	-	expression tag	UNP Q57XD5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP Q57XD5
B	-10	HIS	-	expression tag	UNP Q57XD5
B	-9	SER	-	expression tag	UNP Q57XD5
B	-8	SER	-	expression tag	UNP Q57XD5
B	-7	GLY	-	expression tag	UNP Q57XD5
B	-6	LEU	-	expression tag	UNP Q57XD5
B	-5	VAL	-	expression tag	UNP Q57XD5
B	-4	PRO	-	expression tag	UNP Q57XD5
B	-3	ARG	-	expression tag	UNP Q57XD5
B	-2	GLY	-	expression tag	UNP Q57XD5
B	-1	SER	-	expression tag	UNP Q57XD5
B	0	HIS	-	expression tag	UNP Q57XD5
B	337	ALA	CYS	engineered mutation	UNP Q57XD5
C	-15	HIS	-	expression tag	UNP Q57XD5
C	-14	HIS	-	expression tag	UNP Q57XD5
C	-13	HIS	-	expression tag	UNP Q57XD5
C	-12	HIS	-	expression tag	UNP Q57XD5
C	-11	HIS	-	expression tag	UNP Q57XD5
C	-10	HIS	-	expression tag	UNP Q57XD5
C	-9	SER	-	expression tag	UNP Q57XD5
C	-8	SER	-	expression tag	UNP Q57XD5
C	-7	GLY	-	expression tag	UNP Q57XD5
C	-6	LEU	-	expression tag	UNP Q57XD5
C	-5	VAL	-	expression tag	UNP Q57XD5
C	-4	PRO	-	expression tag	UNP Q57XD5
C	-3	ARG	-	expression tag	UNP Q57XD5
C	-2	GLY	-	expression tag	UNP Q57XD5
C	-1	SER	-	expression tag	UNP Q57XD5
C	0	HIS	-	expression tag	UNP Q57XD5
C	337	ALA	CYS	engineered mutation	UNP Q57XD5
D	-15	HIS	-	expression tag	UNP Q57XD5
D	-14	HIS	-	expression tag	UNP Q57XD5
D	-13	HIS	-	expression tag	UNP Q57XD5
D	-12	HIS	-	expression tag	UNP Q57XD5
D	-11	HIS	-	expression tag	UNP Q57XD5
D	-10	HIS	-	expression tag	UNP Q57XD5
D	-9	SER	-	expression tag	UNP Q57XD5
D	-8	SER	-	expression tag	UNP Q57XD5
D	-7	GLY	-	expression tag	UNP Q57XD5
D	-6	LEU	-	expression tag	UNP Q57XD5
D	-5	VAL	-	expression tag	UNP Q57XD5
D	-4	PRO	-	expression tag	UNP Q57XD5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ARG	-	expression tag	UNP Q57XD5
D	-2	GLY	-	expression tag	UNP Q57XD5
D	-1	SER	-	expression tag	UNP Q57XD5
D	0	HIS	-	expression tag	UNP Q57XD5
D	337	ALA	CYS	engineered mutation	UNP Q57XD5

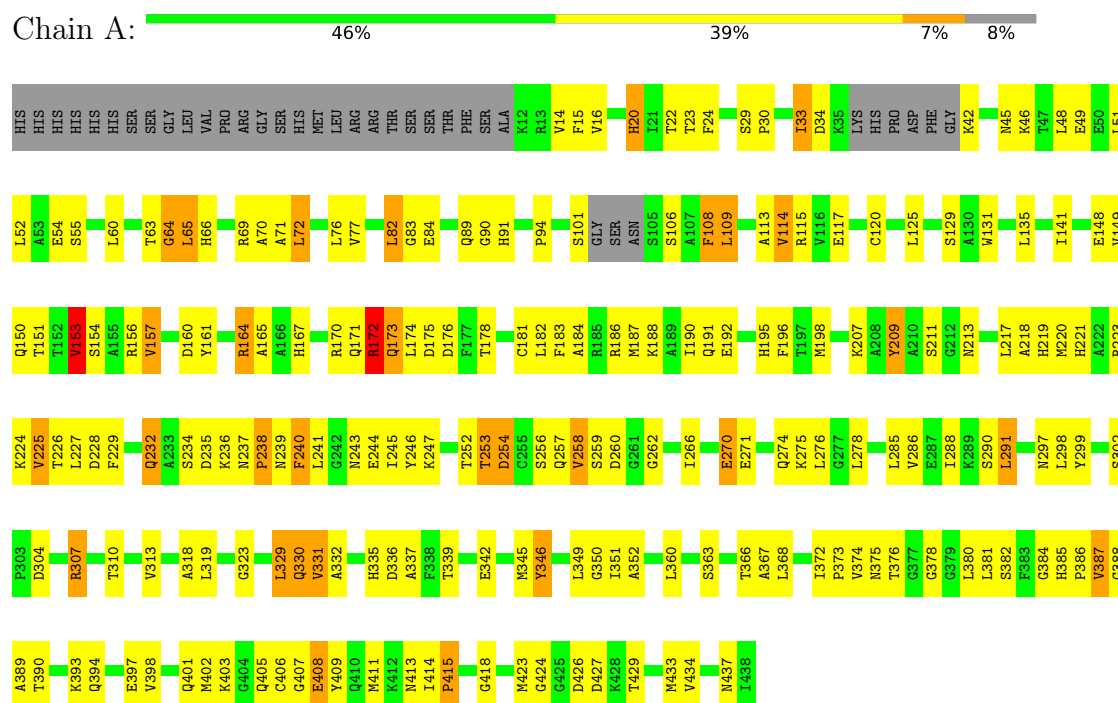
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total O 5 5	0	0
2	B	1	Total O 1 1	0	0
2	C	8	Total O 8 8	0	0
2	D	14	Total O 14 14	0	0

3 Residue-property plots

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.

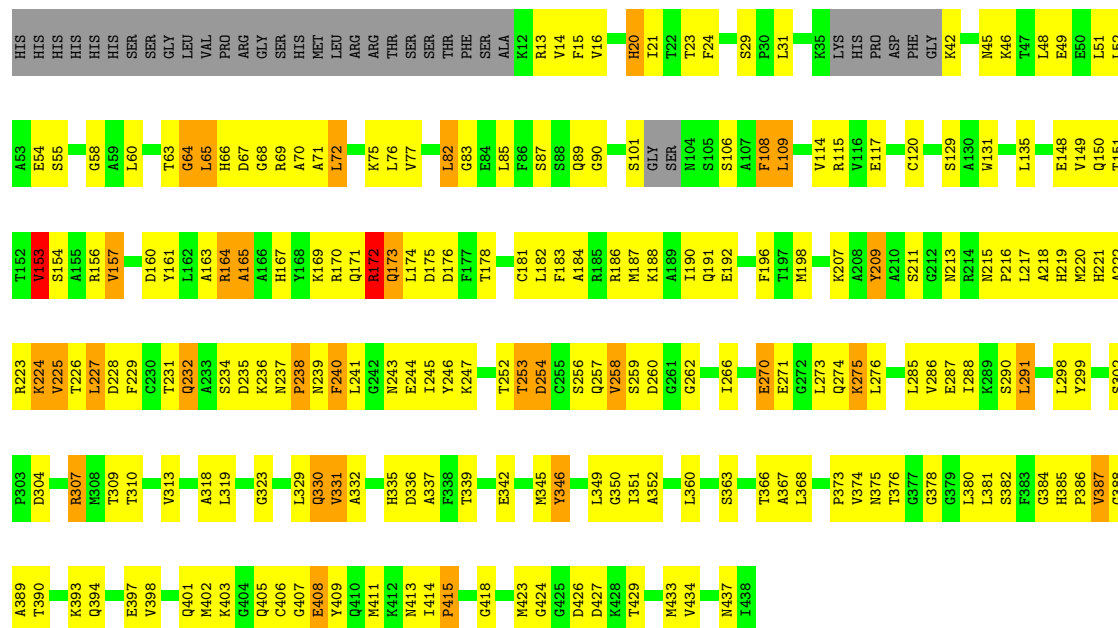
• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE





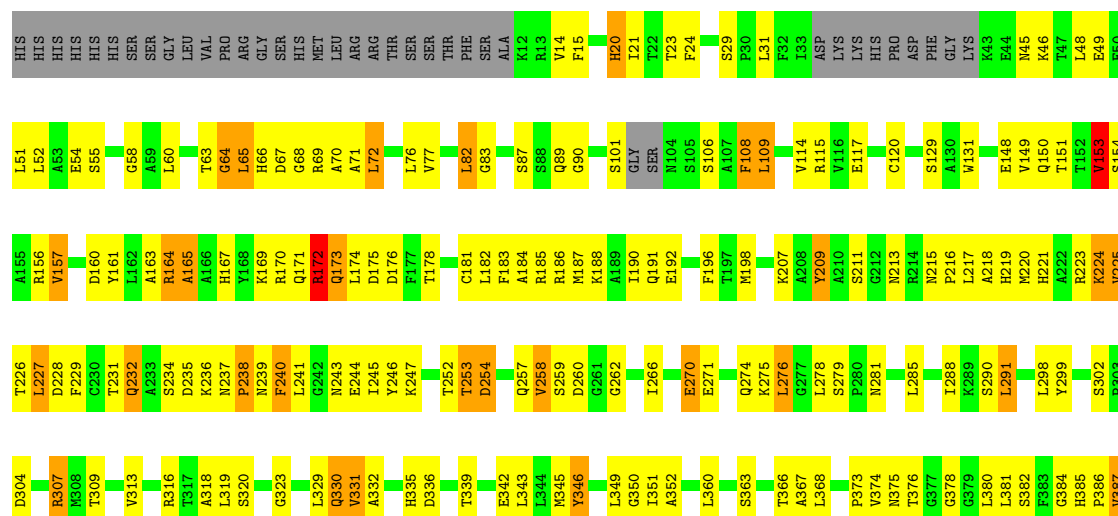
• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE

Chain C: 45% 40% 7% 8%



• Molecule 1: 3-KETOACYL-COA THIOLASE, PUTATIVE

Chain D: 46% 38% 7% 8%



G388	A389	T390	K393	Q394	E397	V398	Q401	M402	K403	G404	Q405	C406	G407	E408	Y409	Q410	M411	K412	N413	I414	P415	G418	M423	G424	G425	D426	D427	K428	T429	M433	V434	M437	I438
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	60.13Å 60.13Å 375.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.36 – 2.90 37.36 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.36-2.90) 92.1 (37.36-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.267 , 0.296 0.254 , 0.265	Depositor DCC
R_{free} test set	1704 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 151.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.438 for -h,-k,l 0.440 for h,-h-k,-l 0.448 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 33651 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12319	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.38	0/3118	0.89	6/4217 (0.1%)
1	B	0.41	0/3114	0.96	11/4210 (0.3%)
1	C	0.38	0/3133	0.90	7/4238 (0.2%)
1	D	0.39	0/3111	0.93	9/4206 (0.2%)
All	All	0.39	0/12476	0.92	33/16871 (0.2%)

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	185	ARG	NE-CZ-NH2	-12.05	108.35	119.20
1	B	164	ARG	NE-CZ-NH2	-11.79	108.59	119.20
1	B	164	ARG	NE-CZ-NH1	11.61	133.11	121.50
1	D	185	ARG	NE-CZ-NH1	10.88	132.38	121.50
1	B	307	ARG	NE-CZ-NH1	10.45	131.95	121.50

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	3072	0	3058	150	1
1	B	3068	0	3067	153	0
1	C	3086	0	3076	155	0
1	D	3065	0	3063	148	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	1	0	0	0	0
2	C	8	0	0	0	0
2	D	14	0	0	0	0
All	All	12319	0	12264	591	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 24.

The worst 5 of 591 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:C:20:HIS:HD2	1:C:58:GLY:HA3	1.40	0.85
1:B:51:LEU:HD21	1:B:260:ASP:HB3	1.58	0.84
1:D:20:HIS:HD2	1:D:58:GLY:HA3	1.43	0.82
1:C:403:LYS:HE3	1:C:437:ASN:HD21	1.45	0.81
1:D:403:LYS:HE3	1:D:437:ASN:HD21	1.45	0.80

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:A:30:PRO:O	1:D:224:LYS:NZ[2_425]	2.17	0.03

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	412/454 (91%)	341 (83%)	53 (13%)	18 (4%)	2 8
1	B	410/454 (90%)	338 (82%)	54 (13%)	18 (4%)	2 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	415/454 (91%)	341 (82%)	56 (14%)	18 (4%)	2	8
1	D	410/454 (90%)	338 (82%)	54 (13%)	18 (4%)	2	8
All	All	1647/1816 (91%)	1358 (82%)	217 (13%)	72 (4%)	2	8

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ALA
1	A	108	PHE
1	A	387	VAL
1	B	71	ALA
1	B	105	SER

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	314/349 (90%)	285 (91%)	29 (9%)	8	27
1	B	315/349 (90%)	285 (90%)	30 (10%)	8	26
1	C	316/349 (90%)	287 (91%)	29 (9%)	8	27
1	D	314/349 (90%)	286 (91%)	28 (9%)	9	28
All	All	1259/1396 (90%)	1143 (91%)	116 (9%)	8	27

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	405	GLN
1	D	330	GLN
1	C	224	LYS
1	D	329	LEU
1	D	225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	437	ASN
1	D	191	GLN
1	D	437	ASN
1	D	221	HIS
1	D	128	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 oligosaccharides 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	418/454 (92%)	-1.13	0 100 100	28, 68, 94, 122	0
1	B	416/454 (91%)	-1.10	0 100 100	28, 67, 95, 123	0
1	C	419/454 (92%)	-1.11	0 100 100	29, 67, 95, 121	0
1	D	416/454 (91%)	-1.12	0 100 100	30, 66, 95, 121	0
All	All	1669/1816 (91%)	-1.12	0 100 100	28, 67, 95, 123	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.