W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2020 – 08:14 PM BST

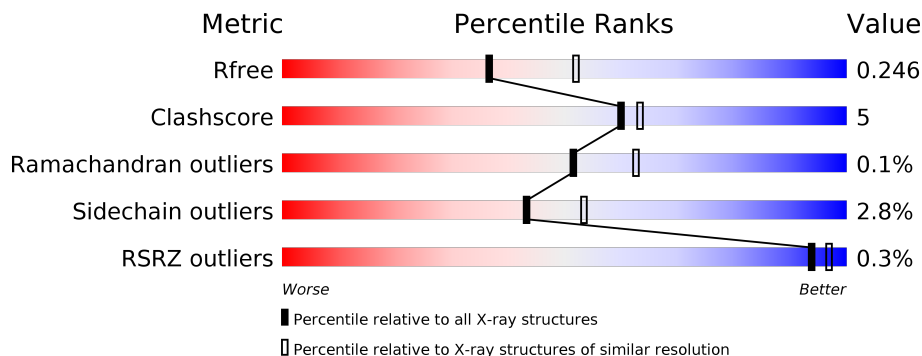|		
PDB ID	:	3R9A
Title	:	Human alanine-glyoxylate aminotransferase in complex with the TPR domain of human PEX5P
Authors	:	Fodor, K.; Wilmanns, M.
Deposited on	:	2011-03-25
Resolution	:	2.35 Å(reported)

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 2.35 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		2.8%
RSRZ outliers		0.3%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	394	87%　　　　10%　··
1	C	394	88%　　　　10%　··
2	B	328	% 79%　　　8%　·　12%
2	D	328	79%　　　9%　·　11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11436 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 Serine–pyruvate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	387	Total 2999	C 1917	N 520	O 545	P 1	S 16	0	1	0
1	C	389	Total 3014	C 1925	N 525	O 546	P 1	S 17	0	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P21549
A	0	ALA	-	EXPRESSION TAG	UNP P21549
C	-1	GLY	-	EXPRESSION TAG	UNP P21549
C	0	ALA	-	EXPRESSION TAG	UNP P21549

- Molecule 2 is a protein called Peroxisomal targeting signal 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	289	Total 2274	C 1427	N 399	O 437	S 11	0	1	0
2	D	292	Total 2304	C 1452	N 400	O 441	S 11	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	312	GLY	-	EXPRESSION TAG	UNP P50542
B	313	ALA	-	EXPRESSION TAG	UNP P50542
B	314	MET	-	EXPRESSION TAG	UNP P50542
D	312	GLY	-	EXPRESSION TAG	UNP P50542
D	313	ALA	-	EXPRESSION TAG	UNP P50542
D	314	MET	-	EXPRESSION TAG	UNP P50542

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN

E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).
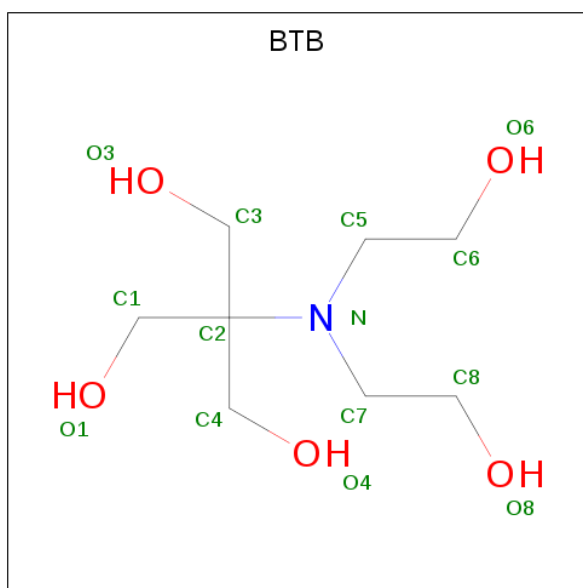
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	307	Total 307	O 307	0	0
4	B	186	Total 186	O 186	0	0
4	C	204	Total 204	O 204	0	0
4	D	134	Total 134	O 134	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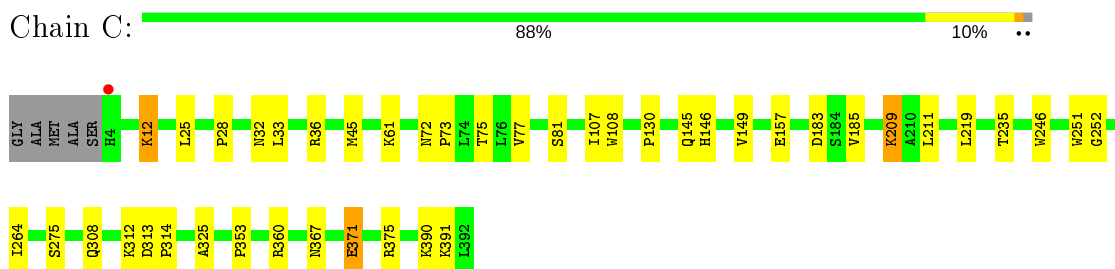 graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above 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.

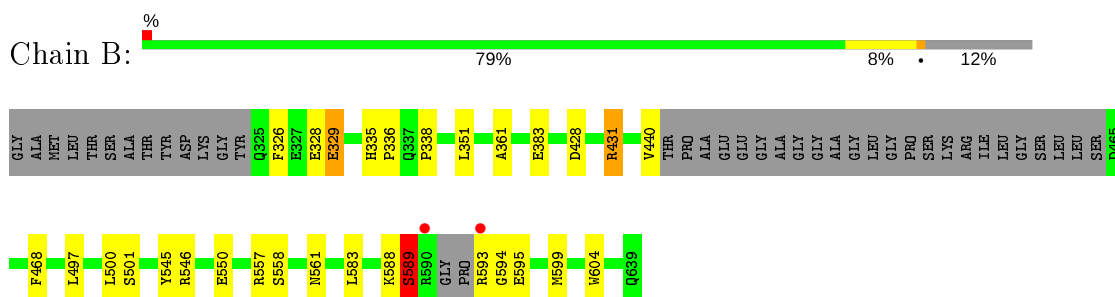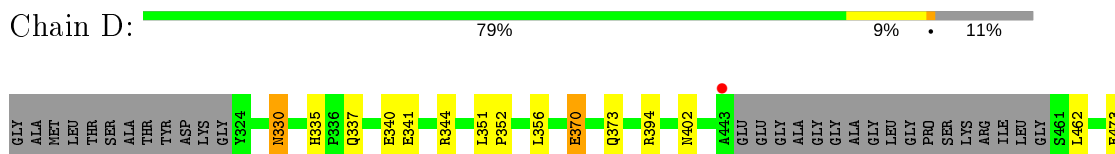- Molecule 1: Serine–pyruvate aminotransferase
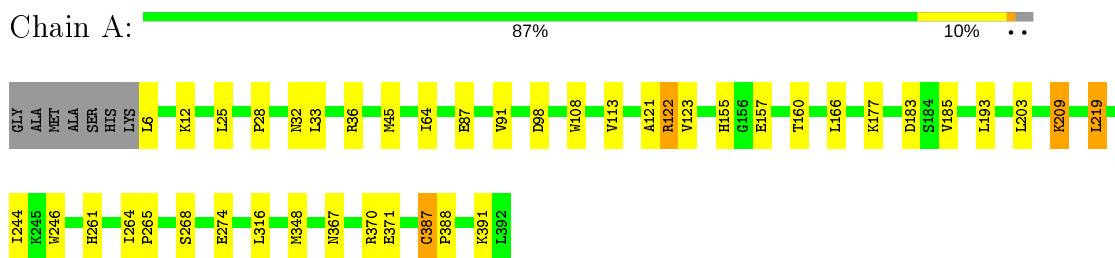
Chain A:

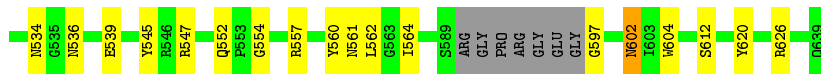- Molecule 1: Serine–pyruvate aminotransferase

Chain C:

- Molecule 2: Peroxisomal targeting signal 1 receptor

Chain B:

- Molecule 2: Peroxisomal targeting signal 1 receptor

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.37Å 99.16Å 127.70Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	78.09 – 2.35 78.12 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (78.09-2.35) 99.6 (78.12-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.77 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.184 , 0.239 0.191 , 0.246	Depositor DCC
R_{free} test set	3096 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.3	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11436	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.46% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, BTB

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	0.42	0/3045	0.57	0/4130
1	C	0.38	0/3065	0.54	0/4161
2	B	0.44	0/2319	0.54	0/3141
2	D	0.41	0/2354	0.53	0/3193
All	All	0.41	0/10783	0.55	0/14625

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	329	GLU	Peptide

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	2999	0	3036	28	0
1	C	3014	0	3026	30	0
2	B	2274	0	2217	23	0
2	D	2304	0	2261	22	0
3	C	14	0	19	2	0
4	A	307	0	0	4	0
4	B	186	0	0	0	0
4	C	204	0	0	1	0
4	D	134	0	0	4	0
All	All	11436	0	10559	97	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 5.

The worst 5 of 97 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:LEU:H	1:A:32:ASN:HD21	1.24	0.86
2:B:583:LEU:HB3	2:B:599:MET:HE3	1.57	0.85
2:B:588:LYS:HA	2:B:589:SER:HB2	1.58	0.84
2:D:552:GLN:HE21	2:D:554:GLY:H	1.25	0.81
1:C:183:ASP:OD1	1:C:209:LLP:H2'2	1.86	0.76

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	385/394 (98%)	377 (98%)	7 (2%)	1 (0%)	41	47
1	C	389/394 (99%)	380 (98%)	9 (2%)	0	100	100
2	B	284/328 (87%)	279 (98%)	4 (1%)	1 (0%)	34	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	288/328 (88%)	282 (98%)	6 (2%)	0	100	100
All	All	1346/1444 (93%)	1318 (98%)	26 (2%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	589	SER
1	A	387	CYS

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	319/325 (98%)	311 (98%)	8 (2%)	47	58
1	C	317/325 (98%)	308 (97%)	9 (3%)	43	53
2	B	238/264 (90%)	233 (98%)	5 (2%)	53	65
2	D	244/264 (92%)	234 (96%)	10 (4%)	30	37
All	All	1118/1178 (95%)	1086 (97%)	32 (3%)	43	52

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	36	ARG
1	C	219	LEU
2	D	539	GLU
1	C	157	GLU
1	C	235	THR

Some 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	72	ASN
1	C	261	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	419	GLN
1	C	32	ASN
2	D	536	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#|Z| > 2$
1	LLP	A	209	1	23,24,25	1.86	5 (21%)	25,32,34	1.68	5 (20%)
1	LLP	C	209	1	23,24,25	1.91	6 (26%)	25,32,34	2.26	6 (24%)

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
1	LLP	A	209	1	-	5/16/17/19	0/1/1/1
1	LLP	C	209	1	-	2/16/17/19	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	LLP	O3-C3	-5.87	1.23	1.37
1	C	209	LLP	O3-C3	-5.70	1.23	1.37
1	C	209	LLP	C2-N1	3.47	1.40	1.33
1	C	209	LLP	C4-C4'	3.29	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	LLP	C2-N1	3.12	1.39	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	LLP	OP4-C5'-C5	8.54	125.63	109.35
1	A	209	LLP	OP4-C5'-C5	4.95	118.78	109.35
1	C	209	LLP	C5-C6-N1	-3.41	118.15	123.82
1	A	209	LLP	CE-NZ-C4'	-3.04	109.57	118.90
1	C	209	LLP	CE-NZ-C4'	-2.69	110.66	118.90

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	209	LLP	C4-C4'-NZ-CE
1	A	209	LLP	O-C-CA-CB
1	C	209	LLP	C4-C4'-NZ-CE
1	C	209	LLP	O-C-CA-CB
1	A	209	LLP	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	209	LLP	3	0
1	C	209	LLP	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	BTB	C	393	-	13,13,13	0.41	0	7,16,16	0.39	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	BTB	C	393	-	-	6/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	393	BTB	C1-C2-N-C5
3	C	393	BTB	C3-C2-N-C5
3	C	393	BTB	C4-C2-N-C5
3	C	393	BTB	N-C5-C6-O6
3	C	393	BTB	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	393	BTB	2	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, 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	386/394 (97%)	-0.34	0	100	100	16, 26, 39, 52	0
1	C	388/394 (98%)	-0.29	1 (0%)	94	97	20, 32, 47, 57	0
2	B	289/328 (88%)	-0.29	2 (0%)	87	92	18, 28, 42, 63	0
2	D	292/328 (89%)	-0.15	1 (0%)	94	97	21, 36, 57, 73	0
All	All	1355/1444 (93%)	-0.27	4 (0%)	94	97	16, 30, 49, 73	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	443	ALA	3.2
1	C	4	HIS	2.6
2	B	590	ARG	2.3
2	B	593	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th 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(Å^2)	Q<0.9
1	LLP	C	209	24/25	0.92	0.20	24,34,42,43	0
1	LLP	A	209	24/25	0.94	0.18	21,35,39,40	0

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, 95th 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(Å^2)	Q<0.9
3	BTB	C	393	14/14	0.85	0.21	59,61,61,63	0

6.5 Other polymers (i)

There are no such residues in this entry.