



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 05:44 PM EDT

PDB ID : 6RUE  
Title : Wolinella succinogenes L-asparaginase mutant V23Q,K24T with L-Asp  
Authors : Timofeev, V.I.; Kuranova, I.P.  
Deposited on : 2019-05-28  
Resolution : 1.65 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](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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

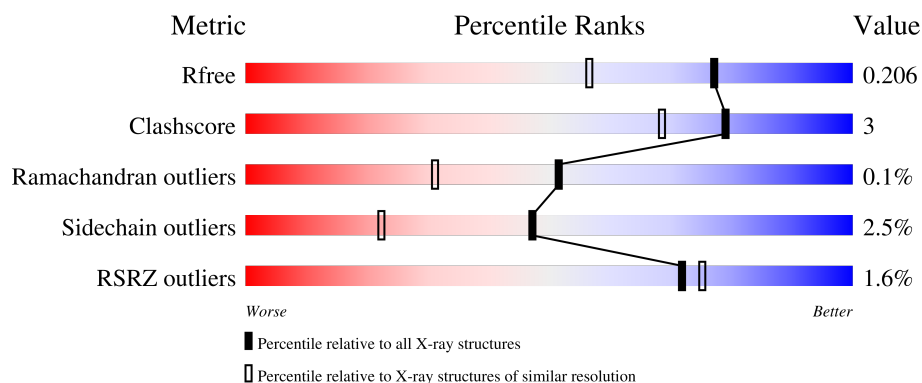
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	318	<div> <div style="width: 93%;"></div> <div style="width: 7%;"></div> </div>
2	B	314	<div> <div style="width: 91%;"></div> <div style="width: 8%;"></div> </div>
3	C	315	<div> <div style="width: 93%;"></div> <div style="width: 6%;"></div> </div>
4	D	317	<div> <div style="width: 92%;"></div> <div style="width: 8%;"></div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10218 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 L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2363	1484	407	464	8			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P50286
A	?	-	GLU	deletion	UNP P50286
A	?	-	SER	deletion	UNP P50286
A	?	-	SER	deletion	UNP P50286
A	?	-	VAL	deletion	UNP P50286
A	?	-	LYS	deletion	UNP P50286
A	?	-	SER	deletion	UNP P50286
A	?	-	SER	deletion	UNP P50286
A	?	-	TYR	deletion	UNP P50286
A	?	-	SER	deletion	UNP P50286
A	121	PRO	SER	conflict	UNP P50286

- Molecule 2 is a protein called L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	314	Total	C	N	O	S	0	0	0
			2343	1473	403	459	8			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P50286
B	?	-	GLY	deletion	UNP P50286
B	?	-	GLU	deletion	UNP P50286
B	?	-	SER	deletion	UNP P50286
B	?	-	SER	deletion	UNP P50286

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	deletion	UNP P50286
B	?	-	LYS	deletion	UNP P50286
B	?	-	SER	deletion	UNP P50286
B	?	-	SER	deletion	UNP P50286
B	?	-	TYR	deletion	UNP P50286
B	?	-	SER	deletion	UNP P50286
B	?	-	ALA	deletion	UNP P50286
B	?	-	GLY	deletion	UNP P50286
B	?	-	ALA	deletion	UNP P50286
B	121	PRO	SER	conflict	UNP P50286

- Molecule 3 is a protein called L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	315	Total	C	N	O	S	0	0	0
			2348	1476	404	460	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP P50286
C	?	-	GLY	deletion	UNP P50286
C	?	-	GLU	deletion	UNP P50286
C	?	-	SER	deletion	UNP P50286
C	?	-	SER	deletion	UNP P50286
C	?	-	VAL	deletion	UNP P50286
C	?	-	LYS	deletion	UNP P50286
C	?	-	SER	deletion	UNP P50286
C	?	-	SER	deletion	UNP P50286
C	?	-	TYR	deletion	UNP P50286
C	?	-	SER	deletion	UNP P50286
C	?	-	ALA	deletion	UNP P50286
C	?	-	GLY	deletion	UNP P50286
C	121	PRO	SER	conflict	UNP P50286

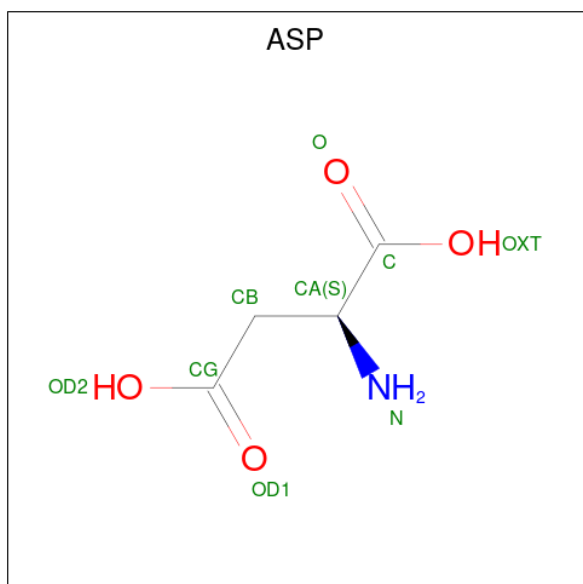
- Molecule 4 is a protein called L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	317	Total	C	N	O	S	0	0	0
			2358	1481	406	463	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLU	deletion	UNP P50286
D	?	-	SER	deletion	UNP P50286
D	?	-	SER	deletion	UNP P50286
D	?	-	VAL	deletion	UNP P50286
D	?	-	LYS	deletion	UNP P50286
D	?	-	SER	deletion	UNP P50286
D	?	-	SER	deletion	UNP P50286
D	?	-	TYR	deletion	UNP P50286
D	?	-	SER	deletion	UNP P50286
D	?	-	ALA	deletion	UNP P50286
D	?	-	GLY	deletion	UNP P50286
D	121	PRO	SER	conflict	UNP P50286

- Molecule 5 is ASPARTIC ACID (three-letter code: ASP) (formula:  $C_4H_7NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	4	1	4		
5	B	1	Total	C	N	O	0	0
			9	4	1	4		
5	C	1	Total	C	N	O	0	0
			9	4	1	4		
5	D	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	217	Total 217	O 217	0	0
6	B	192	Total 192	O 192	0	0
6	C	185	Total 185	O 185	0	0
6	D	176	Total 176	O 176	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: L-asparaginase

Chain A: 

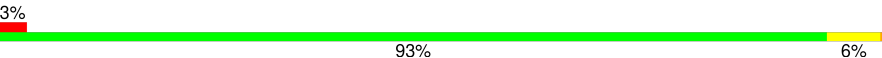


- Molecule 2: L-asparaginase

Chain B: 

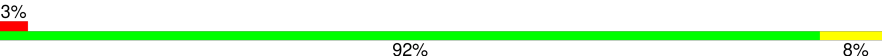


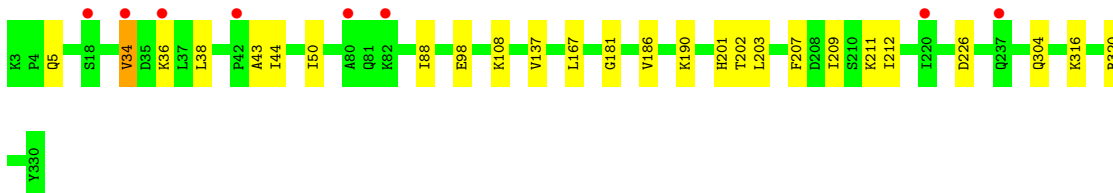
- Molecule 3: L-asparaginase

Chain C: 



- Molecule 4: L-asparaginase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.92Å 134.36Å 73.15Å 90.00° 93.70° 90.00°	Depositor
Resolution (Å)	30.00 – 1.65 29.82 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-1.65) 97.5 (29.82-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.169 , 0.200 0.178 , 0.206	Depositor DCC
$R_{free}$ test set	7333 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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](#)

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	0.77	1/2394 (0.0%)	0.87	0/3245
2	B	0.76	1/2374 (0.0%)	0.88	0/3218
3	C	0.76	0/2379	0.91	1/3225 (0.0%)
4	D	0.76	0/2389	0.86	0/3238
All	All	0.76	2/9536 (0.0%)	0.88	1/12926 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	321	GLU	CD-OE1	5.55	1.31	1.25
1	A	321	GLU	CD-OE1	5.47	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	320	ARG	NE-CZ-NH1	6.28	123.44	120.30

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	2363	0	2424	12	0
2	B	2343	0	2406	16	0
3	C	2348	0	2411	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2358	0	2419	13	0
5	A	9	0	3	0	0
5	B	9	0	3	0	0
5	C	9	0	3	2	0
5	D	9	0	3	0	0
6	A	217	0	0	3	0
6	B	192	0	0	1	0
6	C	185	0	0	3	0
6	D	176	0	0	2	0
All	All	10218	0	9672	54	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 3.

The worst 5 of 54 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)
3:C:38:LEU:HD23	3:C:44:ILE:HD11	1.17	1.15
3:C:3:LYS:N	6:C:501:HOH:O	1.91	1.01
3:C:38:LEU:CD2	3:C:44:ILE:HD11	1.91	0.99
6:A:692:HOH:O	3:C:14:THR:HG21	1.87	0.73
3:C:5:GLN:HG2	6:C:542:HOH:O	1.91	0.70

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	314/318 (99%)	305 (97%)	9 (3%)	0	100	100
2	B	310/314 (99%)	301 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	311/315 (99%)	301 (97%)	10 (3%)	0	100	100
4	D	313/317 (99%)	301 (96%)	11 (4%)	1 (0%)	41	22
All	All	1248/1264 (99%)	1208 (97%)	39 (3%)	1 (0%)	51	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	43	ALA

### 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	255/255 (100%)	249 (98%)	6 (2%)	49	23
2	B	254/254 (100%)	248 (98%)	6 (2%)	49	23
3	C	254/254 (100%)	247 (97%)	7 (3%)	43	18
4	D	255/255 (100%)	248 (97%)	7 (3%)	44	19
All	All	1018/1018 (100%)	992 (97%)	26 (3%)	47	21

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	36	LYS
3	C	203	LEU
4	D	226	ASP
3	C	38	LEU
3	C	316	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	81	GLN

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Mol	Chain	Res	Type
4	D	201	HIS
3	C	110	GLN
4	D	259	ASN
4	D	81	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z  > 2$
5	ASP	C	400	-	7,8,8	0.96	1 (14%)	6,10,10	1.52	2 (33%)
5	ASP	D	400	-	7,8,8	0.94	0	6,10,10	0.62	0
5	ASP	A	400	-	7,8,8	1.13	0	6,10,10	1.71	2 (33%)
5	ASP	B	400	-	7,8,8	0.99	0	6,10,10	1.20	1 (16%)

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
5	ASP	C	400	-	-	4/8/8/8	-
5	ASP	D	400	-	-	2/8/8/8	-
5	ASP	A	400	-	-	2/8/8/8	-
5	ASP	B	400	-	-	4/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	400	ASP	OXT-C	-2.23	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	400	ASP	OD1-CG-CB	-2.66	114.68	122.84
5	C	400	ASP	OD1-CG-CB	-2.48	115.22	122.84
5	A	400	ASP	OD2-CG-CB	2.22	120.89	114.00
5	C	400	ASP	OD2-CG-CB	2.21	120.88	114.00
5	B	400	ASP	OD1-CG-CB	-2.19	116.11	122.84

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	400	ASP	O-C-CA-N
5	D	400	ASP	O-C-CA-N
5	A	400	ASP	OXT-C-CA-N
5	C	400	ASP	OXT-C-CA-N
5	B	400	ASP	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	400	ASP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
4	D	1
3	C	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	17:GLY	C	28:SER	N	17.13
1	D	19:GLY	C	31:ALA	N	9.05
1	C	17:GLY	C	31:ALA	N	6.49
1	B	17:GLY	C	32:VAL	N	5.48

## 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	318/318 (100%)	-0.22	0 100 100	10, 14, 26, 35	0
2	B	314/314 (100%)	-0.09	4 (1%) 77 80	10, 16, 35, 59	0
3	C	315/315 (100%)	-0.01	8 (2%) 57 58	10, 16, 34, 58	0
4	D	317/317 (100%)	0.04	8 (2%) 57 58	11, 17, 38, 53	0
All	All	1264/1264 (100%)	-0.07	20 (1%) 72 75	10, 16, 34, 59	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	31	ALA	5.4
3	C	33	THR	5.1
3	C	38	LEU	4.5
2	B	33	THR	4.3
4	D	42	PRO	4.0

### 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](#)

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
5	ASP	A	400	9/9	0.93	0.11	12,20,28,30	0
5	ASP	B	400	9/9	0.97	0.07	13,14,15,16	0
5	ASP	C	400	9/9	0.98	0.06	13,16,17,18	0
5	ASP	D	400	9/9	0.98	0.07	12,14,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.