Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2025 – 03:08 pm GMT

PDB ID	:	8RJ0
Title	:	Crystal structure of mutant aspartase from Bacillus sp. YM55-1 in the closed loop conformation
Authors	:	Capra, N.; Thunnissen, A.M.W.H.; Janssen, D.B.
Deposited on	:	2023-12-19
Resolution	:	1.90 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 ⓘ 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:

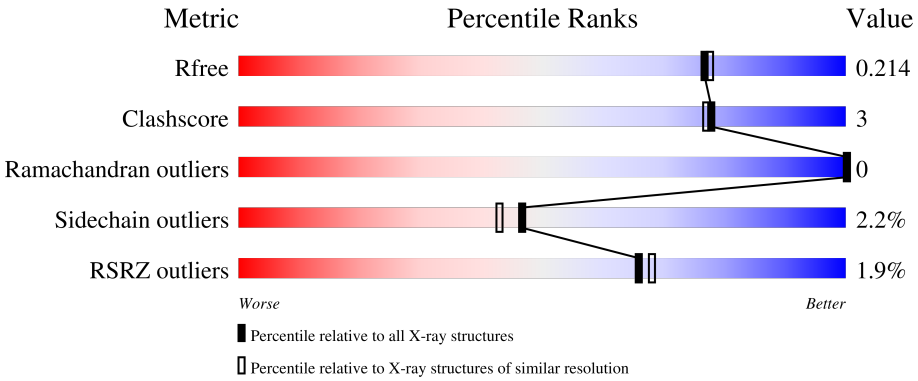
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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 <=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	468	3% 89% 9%
1	B	468	% 91% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7375 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.

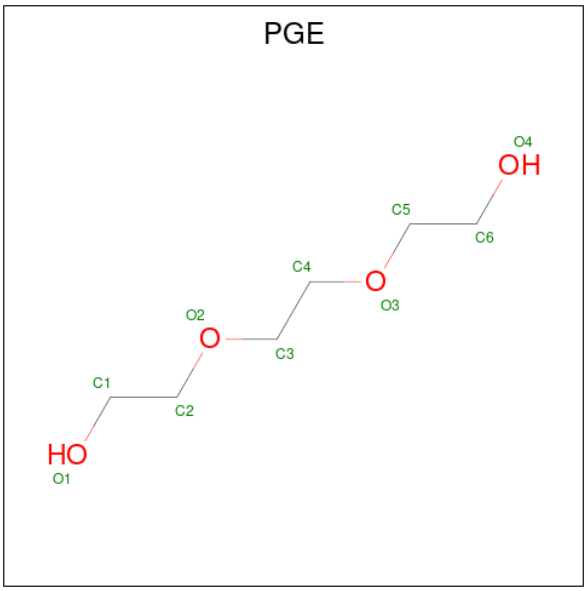
- Molecule 1 is a protein called Aspartate ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	2	0
			3578	2255	607	693	23			
1	B	463	Total	C	N	O	S	0	0	0
			3571	2253	603	692	23			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	ILE	THR	engineered mutation	UNP Q9LCC6
A	321	ILE	MET	engineered mutation	UNP Q9LCC6
A	324	MET	LYS	engineered mutation	UNP Q9LCC6
A	326	CYS	ASN	engineered mutation	UNP Q9LCC6
A	422	SER	ALA	engineered mutation	UNP Q9LCC6
A	429	ASP	TYR	engineered mutation	UNP Q9LCC6
A	460	ILE	THR	conflict	UNP Q9LCC6
B	187	ILE	THR	engineered mutation	UNP Q9LCC6
B	321	ILE	MET	engineered mutation	UNP Q9LCC6
B	324	MET	LYS	engineered mutation	UNP Q9LCC6
B	326	CYS	ASN	engineered mutation	UNP Q9LCC6
B	422	SER	ALA	engineered mutation	UNP Q9LCC6
B	429	ASP	TYR	engineered mutation	UNP Q9LCC6
B	460	ILE	THR	conflict	UNP Q9LCC6

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0

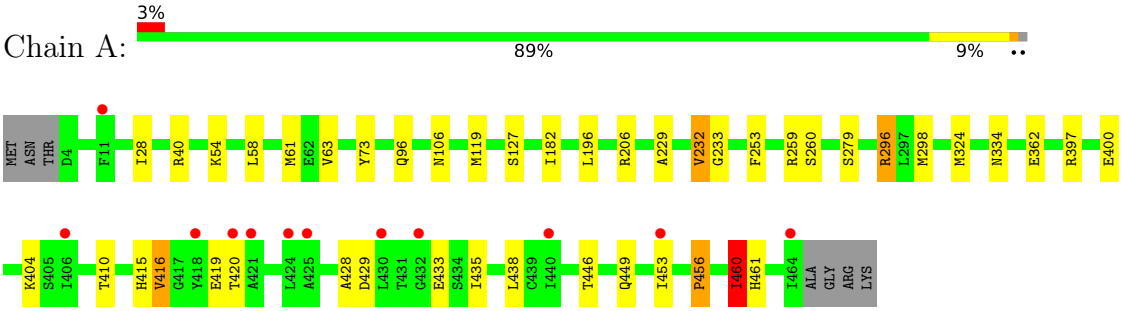
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	103	Total O 105 105	0	2
4	B	109	Total O 109 109	0	0

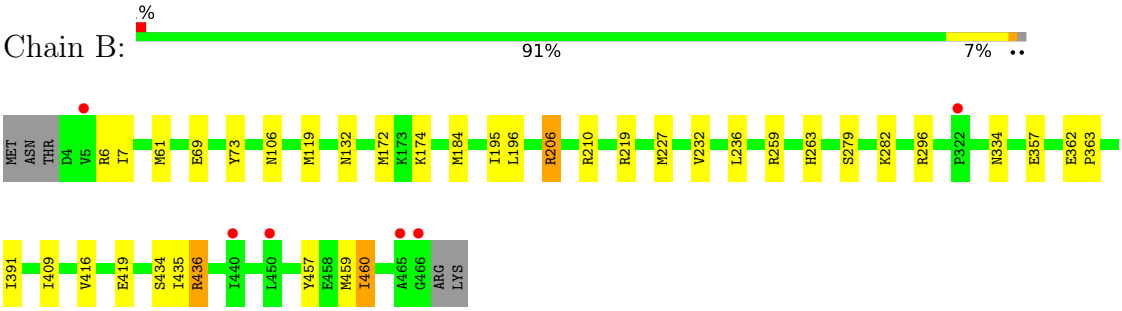
3 Residue-property plots (i)

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: Aspartate ammonia-lyase



• Molecule 1: Aspartate ammonia-lyase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	75.87Å 98.99Å 136.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.57 – 1.90 46.57 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.57-1.90) 99.0 (46.57-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.169 , 0.207 0.179 , 0.214	Depositor DCC
R_{free} test set	4215 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.8	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	0.97	EDS
Total number of atoms	7375	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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

5.1 Standard geometry

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

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	0.65	1/3636 (0.0%)	1.02	10/4920 (0.2%)
1	B	0.67	0/3629	1.05	12/4911 (0.2%)
All	All	0.66	1/7265 (0.0%)	1.04	22/9831 (0.2%)

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
1	A	0	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	GLU	CD-OE1	5.73	1.31	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	227	MET	CG-SD-CE	-9.66	84.74	100.20
1	A	40	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	B	172	MET	CG-SD-CE	7.61	112.37	100.20
1	A	397	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	B	282	LYS	CD-CE-NZ	7.36	128.64	111.70
1	B	61	MET	CG-SD-CE	6.59	110.75	100.20
1	B	206	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	397	ARG	NE-CZ-NH2	6.15	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	232	VAL	N-CA-CB	-6.15	97.97	111.50
1	B	184	MET	CG-SD-CE	-6.14	90.38	100.20
1	B	210	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	296	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	219	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	324	MET	CG-SD-CE	-5.69	91.10	100.20
1	A	232	VAL	N-CA-CB	-5.55	99.28	111.50
1	A	298	MET	CG-SD-CE	5.51	109.02	100.20
1	B	459	MET	CG-SD-CE	-5.35	91.64	100.20
1	B	69	GLU	N-CA-CB	5.34	120.22	110.60
1	A	416	VAL	N-CA-CB	-5.31	99.83	111.50
1	A	460	ILE	N-CA-CB	-5.29	98.64	110.80
1	B	436	ARG	CD-NE-CZ	5.18	130.85	123.60
1	A	404	LYS	CB-CA-C	-5.04	100.32	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	ARG	Sidechain
1	B	206	ARG	Sidechain
1	B	259	ARG	Sidechain

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	3578	0	3585	26	0
1	B	3571	0	3585	17	0
2	A	10	0	14	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	105	0	0	1	0
4	B	109	0	0	0	0
All	All	7375	0	7184	38	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.

All (38) 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:279:SER:HB3	1:B:279:SER:HB3	1.77	0.67
1:A:449:GLN:O	1:A:453:ILE:HG12	1.97	0.64
1:A:415:HIS:CE1	1:A:453:ILE:HD12	2.35	0.61
1:A:196:LEU:CD1	1:A:460:ILE:HG21	2.32	0.59
1:A:296:ARG:HE	1:A:334:ASN:HD21	1.50	0.58
1:B:296:ARG:HE	1:B:334:ASN:HD21	1.51	0.58
1:A:196:LEU:HG	1:A:460:ILE:HG12	1.86	0.58
1:A:229:ALA:HB1	1:A:233:GLY:HA2	1.86	0.57
1:A:416:VAL:HG13	1:A:420:THR:HB	1.87	0.57
1:B:73:TYR:CD2	1:B:119:MET:HE3	2.38	0.57
1:A:196:LEU:HG	1:A:460:ILE:HG21	1.87	0.56
1:A:196:LEU:HD11	1:A:460:ILE:HG21	1.89	0.53
1:B:196:LEU:HG	1:B:460:ILE:HG12	1.90	0.52
1:A:54:LYS:HE3	1:A:253:PHE:CZ	2.46	0.51
1:A:196:LEU:CG	1:A:460:ILE:HG21	2.41	0.50
1:A:410:THR:HG22	1:B:236:LEU:HD23	1.93	0.49
1:B:416:VAL:CG1	1:B:416:VAL:O	2.60	0.49
1:A:456:PRO:O	1:A:460:ILE:HB	2.14	0.48
1:A:296:ARG:HE	1:A:334:ASN:ND2	2.12	0.47
1:A:206[A]:ARG:HH11	1:B:263:HIS:HB3	1.80	0.47
1:A:433:GLU:HB2	1:A:438:LEU:HD21	1.96	0.47
1:A:232:VAL:HG13	1:B:195:ILE:HD12	1.97	0.46
1:A:182:ILE:HD11	1:A:460:ILE:CD1	2.46	0.46
1:B:6:ARG:C	1:B:7:ILE:HD12	2.36	0.45
1:A:460:ILE:HG22	1:A:461:HIS:HD1	1.82	0.45
1:B:362:GLU:N	1:B:363:PRO:CD	2.79	0.45
1:B:296:ARG:HE	1:B:334:ASN:ND2	2.15	0.45
1:A:96:GLN:NE2	4:A:602:HOH:O	2.46	0.44
1:B:436:ARG:HG3	1:B:436:ARG:HH11	1.82	0.44
1:A:460:ILE:HG22	1:A:461:HIS:ND1	2.33	0.43
1:B:457:TYR:O	1:B:460:ILE:HB	2.18	0.43
1:B:409:ILE:HB	1:B:435:ILE:HG12	1.99	0.43
1:A:206[A]:ARG:NH1	1:B:263:HIS:HB3	2.34	0.42
1:A:58:LEU:HA	1:A:61:MET:HE3	2.02	0.42
1:B:174:LYS:NZ	1:B:391:ILE:O	2.53	0.41
1:A:73:TYR:CD2	1:A:119:MET:HE3	2.55	0.41
1:B:73:TYR:CD2	1:B:119:MET:CE	3.02	0.41
1:A:428:ALA:HB2	1:A:435:ILE:HD13	2.03	0.41

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	461/468 (98%)	454 (98%)	7 (2%)	0	100	100
1	B	461/468 (98%)	454 (98%)	7 (2%)	0	100	100
All	All	922/936 (98%)	908 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	391/395 (99%)	380 (97%)	11 (3%)	38	33
1	B	390/395 (99%)	384 (98%)	6 (2%)	60	59
All	All	781/790 (99%)	764 (98%)	17 (2%)	47	43

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	63	VAL
1	A	106	ASN
1	A	127	SER
1	A	260	SER

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Mol	Chain	Res	Type
1	A	400	GLU
1	A	419	GLU
1	A	429	ASP
1	A	446	THR
1	A	456	PRO
1	A	460	ILE
1	B	106	ASN
1	B	132	ASN
1	B	357	GLU
1	B	419	GLU
1	B	434	SER
1	B	460	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	334	ASN
1	A	355	GLN
1	A	415	HIS
1	A	455	ASN
1	B	96	GLN
1	B	132	ASN
1	B	269	GLN
1	B	334	ASN
1	B	451	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)

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)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
2	PGE	A	501	-	9,9,9	0.46	0	8,8,8	0.36	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
2	PGE	A	501	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PGE	O2-C3-C4-O3
2	A	501	PGE	C3-C4-O3-C5

There are no ring outliers.

No monomer is involved in short contacts.

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

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	461/468 (98%)	0.06	12 (2%) 57 59	20, 43, 74, 115	2 (0%)
1	B	463/468 (98%)	-0.06	6 (1%) 74 76	25, 40, 71, 112	0
All	All	924/936 (98%)	-0.00	18 (1%) 66 68	20, 42, 72, 115	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	464	ILE	5.9
1	B	322	PRO	4.3
1	A	418	TYR	3.3
1	B	450	LEU	3.1
1	A	425	ALA	2.9
1	A	406	ILE	2.9
1	A	11	PHE	2.8
1	A	421	ALA	2.7
1	B	440	ILE	2.6
1	B	466	GLY	2.6
1	A	430	LEU	2.4
1	B	5	VAL	2.4
1	A	424	LEU	2.3
1	A	440	ILE	2.3
1	A	453	ILE	2.3
1	B	465	ALA	2.2
1	A	420	THR	2.1
1	A	432	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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^{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	B-factors(Å^2)	Q<0.9
2	PGE	A	501	10/10	0.93	0.10	41,46,48,51	0
3	NA	A	502	1/1	0.93	0.09	43,43,43,43	1
3	NA	B	501	1/1	0.99	0.05	38,38,38,38	1

6.5 Other polymers (i)

There are no such residues in this entry.