



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 01:29 AM UTC

PDB ID : 1A1E / pdb_00001a1e
Title : C-SRC (SH2 DOMAIN) COMPLEXED WITH ACE-PHOSPHOTYR-GLU-(3-BUTYLPIPERIDINE)
Authors : Shewchuk, L.; Jordan, S.
Deposited on : 1997-12-10
Resolution : 2.20 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

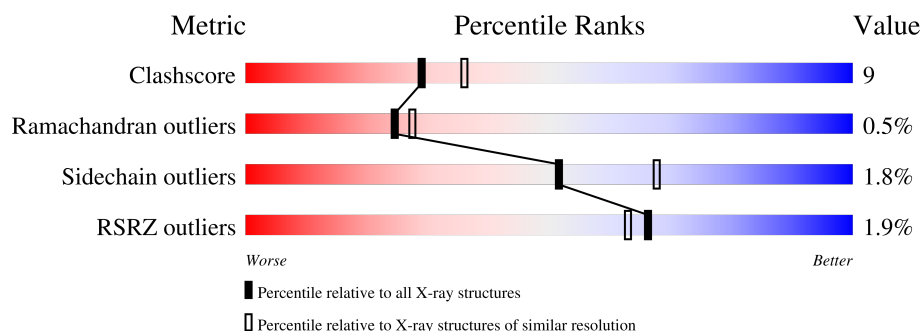
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	107	% 62% 30% 5% ...
1	B	107	3% 63% 30% ...
2	C	4	75% 25%
2	D	4	50% 25% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2245 atoms, of which 486 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 C-SRC TYROSINE KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	104	Total	C	H	N	O	S	0	0	0
			1030	523	201	148	155	3			
1	B	104	Total	C	H	N	O	S	0	0	0
			1003	512	193	145	150	3			

- Molecule 2 is a protein called ACE-PHOSPHOTYR-GLU-(3-BUTYLPIPERIDINE).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	N	O	P	0	0	0
			40	25	2	3	9	1			
2	D	4	Total	C	H	N	O	P	0	0	0
			40	25	2	3	9	1			

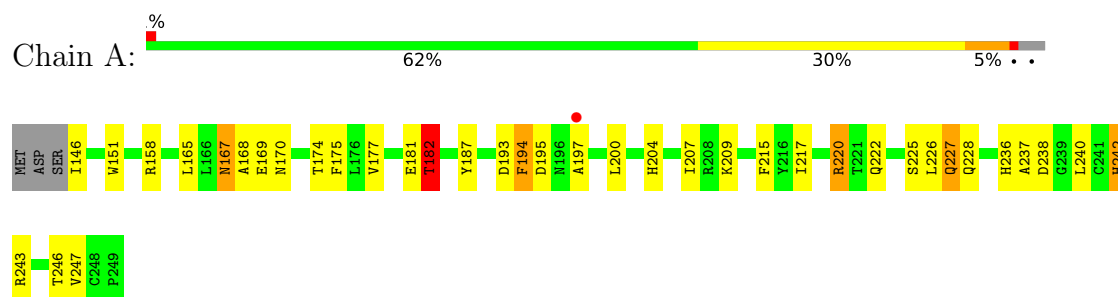
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	25	Total	H	O	0	0
			75	50	25		
3	B	15	Total	H	O	0	0
			45	30	15		
3	C	2	Total	H	O	0	0
			6	4	2		
3	D	2	Total	H	O	0	0
			6	4	2		

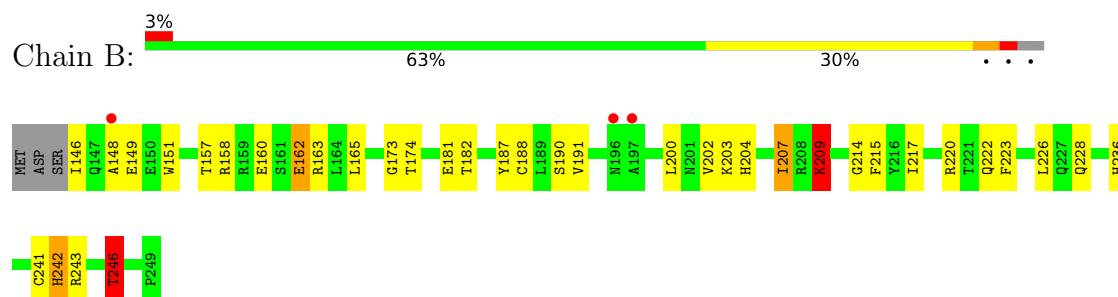
3 Residue-property plots

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.

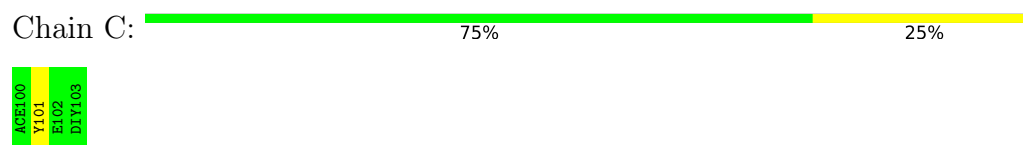
- Molecule 1: C-SRC TYROSINE KINASE



- Molecule 1: C-SRC TYROSINE KINASE



- Molecule 2: ACE-PHOSPHOTYR-GLU-(3-BUTYLPYPERIDINE)



- Molecule 2: ACE-PHOSPHOTYR-GLU-(3-BUTYLPYPERIDINE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.60Å 67.20Å 75.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20 6.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.0 (6.00-2.20) 86.5 (6.00-2.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.192 , (Not available) 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2245	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, DIY, PTR

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	1.15	4/846 (0.5%)	1.91	24/1141 (2.1%)
1	B	1.18	4/827 (0.5%)	1.95	27/1119 (2.4%)
2	C	1.18	0/8	0.96	0/9
2	D	1.07	0/8	1.16	0/9
All	All	1.17	8/1689 (0.5%)	1.92	51/2278 (2.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	HIS	CD2-NE2	-7.26	1.29	1.37
1	B	204	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	242	HIS	CD2-NE2	-6.46	1.30	1.37
1	B	242	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	236	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	236	HIS	CD2-NE2	-5.77	1.31	1.37
1	B	190	SER	CA-CB	-5.63	1.45	1.53
1	A	247	VAL	CA-CB	-5.48	1.48	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	ILE	N-CA-C	-11.38	102.68	111.90
1	A	217	ILE	N-CA-C	-11.19	102.72	112.12
1	B	182	THR	N-CA-C	9.76	121.67	111.14
1	A	170	ASN	CA-C-N	9.46	129.40	119.85
1	A	170	ASN	C-N-CA	9.46	129.40	119.85
1	B	223	PHE	CA-CB-CG	-7.83	105.97	113.80
1	A	151	TRP	CB-CG-CD1	-7.60	115.50	126.90
1	A	167	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	A	220	ARG	CA-CB-CG	-7.48	99.13	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	TRP	CG-CD2-CE3	7.20	141.10	133.90
1	A	165	LEU	N-CA-C	7.19	120.16	111.82
1	B	222	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	B	148	ALA	N-CA-C	6.81	120.27	112.57
1	B	165	LEU	N-CA-C	6.71	120.69	112.23
1	B	246	THR	N-CA-CB	-6.71	99.36	110.23
1	A	194	PHE	O-C-N	6.71	130.67	123.56
1	A	204	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	B	204	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	B	236	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	B	173	GLY	N-CA-C	-6.54	106.04	115.27
1	B	222	GLN	CA-CB-CG	6.53	127.16	114.10
1	A	167	ASN	CB-CG-ND2	6.52	126.19	116.40
1	A	177	VAL	O-C-N	-6.42	116.59	123.14
1	B	181	GLU	CA-C-N	6.32	129.03	120.44
1	B	181	GLU	C-N-CA	6.32	129.03	120.44
1	A	194	PHE	CA-CB-CG	6.22	120.02	113.80
1	B	217	ILE	O-C-N	-6.06	115.77	122.07
1	B	151	TRP	CG-CD2-CE3	6.00	139.90	133.90
1	A	220	ARG	CA-C-O	-5.87	114.65	120.82
1	A	158	ARG	CG-CD-NE	-5.86	99.10	112.00
1	B	151	TRP	CB-CG-CD1	-5.77	118.24	126.90
1	B	246	THR	CB-CA-C	5.70	118.94	109.53
1	B	202	VAL	O-C-N	-5.66	116.93	122.93
1	A	222	GLN	CG-CD-NE2	-5.56	108.06	116.40
1	B	149	GLU	O-C-N	-5.50	116.78	123.16
1	A	182	THR	N-CA-CB	-5.47	101.48	110.40
1	A	236	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	A	181	GLU	CB-CA-C	-5.43	101.62	110.85
1	B	191	VAL	O-C-N	-5.36	117.41	123.20
1	B	162	GLU	CB-CG-CD	5.36	121.71	112.60
1	A	227	GLN	OE1-CD-NE2	-5.34	117.25	122.60
1	B	228	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	A	181	GLU	CA-C-O	5.31	126.05	120.42
1	B	209	LYS	O-C-N	-5.26	117.22	123.22
1	A	151	TRP	CE2-CD2-CG	-5.23	100.93	107.20
1	B	151	TRP	CE2-CD2-CG	-5.18	100.99	107.20
1	A	193	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	220	ARG	CA-CB-CG	-5.13	103.84	114.10
1	A	175	PHE	N-CA-C	5.09	116.73	109.14
1	B	207	ILE	N-CA-C	-5.09	100.24	107.77
1	B	222	GLN	N-CA-C	-5.04	101.71	109.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	829	201	802	16	0
1	B	810	193	768	14	0
2	C	38	2	34	0	0
2	D	38	2	34	2	0
3	A	25	50	0	1	0
3	B	15	30	0	1	0
3	C	2	4	0	0	0
3	D	2	4	0	0	0
All	All	1759	486	1638	29	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 9.

All (29) 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:182:THR:HG23	1:B:163:ARG:HD3	1.58	0.84
1:A:182:THR:HG21	1:B:160:GLU:OE1	1.85	0.76
1:B:146:ILE:CD1	1:B:226:LEU:HD12	2.25	0.66
1:B:242:HIS:HD2	1:B:243:ARG:O	1.81	0.63
1:A:146:ILE:CD1	1:A:226:LEU:HD12	2.29	0.63
1:A:194:PHE:HB3	1:A:200:LEU:HD23	1.83	0.61
1:A:187:TYR:HB2	1:A:207:ILE:HB	1.85	0.59
1:A:209:LYS:HD3	1:A:215:PHE:CE2	2.37	0.58
1:A:242:HIS:HD2	1:A:243:ARG:O	1.87	0.58
1:A:225:SER:HB2	1:A:227:GLN:OE1	2.07	0.54
1:A:182:THR:HG22	3:A:527:HOH:O	2.09	0.52
1:A:167:ASN:OD1	1:A:169:GLU:HG2	2.10	0.51
1:A:225:SER:OG	1:A:228:GLN:HG3	2.12	0.49
1:B:187:TYR:HB2	1:B:207:ILE:HB	1.95	0.49
1:B:174:THR:HA	1:B:246:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASP:OD2	1:A:197:ALA:HB3	2.14	0.48
1:B:209:LYS:HG2	1:B:215:PHE:CE1	2.49	0.48
1:A:167:ASN:HD22	1:A:168:ALA:N	2.13	0.47
1:B:188:CYS:SG	2:D:101:PTR:HE2	2.55	0.46
1:A:220:ARG:NH1	1:A:238:ASP:OD1	2.50	0.44
1:A:174:THR:HA	1:A:246:THR:O	2.18	0.43
1:B:160:GLU:HB3	3:B:512:HOH:O	2.17	0.43
1:B:203:LYS:HD2	1:B:241:CYS:HB3	2.01	0.43
1:B:158:ARG:O	1:B:162:GLU:HG3	2.18	0.43
1:B:146:ILE:HD11	1:B:226:LEU:HD12	2.00	0.42
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.93	0.42
1:A:237:ALA:O	1:A:240:LEU:HG	2.20	0.41
1:B:157:THR:OG1	1:B:160:GLU:HG2	2.20	0.41
2:D:103:DIY:H41	2:D:103:DIY:H2'1	1.85	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	102/107 (95%)	98 (96%)	4 (4%)	0	100	100
1	B	102/107 (95%)	97 (95%)	4 (4%)	1 (1%)	12	11
All	All	204/214 (95%)	195 (96%)	8 (4%)	1 (0%)	24	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	214	GLY

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	87/94 (93%)	86 (99%)	1 (1%)	65	79
1	B	82/94 (87%)	80 (98%)	2 (2%)	43	58
2	C	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
All	All	171/190 (90%)	168 (98%)	3 (2%)	51	68

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	THR
1	B	209	LYS
1	B	246	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	167	ASN
1	A	242	HIS
1	B	228	GLN
1	B	242	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](#)

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
2	PTR	C	101	2	15,16,17	1.07	1 (6%)	17,22,24	0.97	0
2	PTR	D	101	2	15,16,17	1.03	0	17,22,24	0.98	1 (5%)

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	PTR	C	101	2	-	0/10/11/13	0/1/1/1
2	PTR	D	101	2	-	0/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	101	PTR	P-OH	-2.07	1.55	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	101	PTR	O3P-P-O2P	2.13	115.79	107.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	101	PTR	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	104/107 (97%)	-0.55	1 (0%) 79 77	14, 27, 51, 67	0
1	B	104/107 (97%)	-0.47	3 (2%) 53 50	15, 26, 55, 77	0
2	C	1/4 (25%)	-1.27	0 100 100	30, 30, 30, 30	0
2	D	1/4 (25%)	-1.12	0 100 100	37, 37, 37, 37	0
All	All	210/222 (94%)	-0.52	4 (1%) 66 63	14, 27, 55, 77	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	ALA	3.6
1	A	197	ALA	3.2
1	B	148	ALA	2.4
1	B	196	ASN	2.2

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
2	PTR	D	101	16/17	0.94	0.06	0,37,47,52	0
2	PTR	C	101	16/17	0.97	0.05	0,23,29,33	0

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.