

wwPDB X-ray Structure Validation Summary Report (i)

May 19, 2020 – 09:29 pm BST

PDB ID : 2I2W

Title : Crystal Structure of Escherichia Coli Phosphoheptose Isomerase

Authors : DeLeon, G.; Blakely, K.; Zhang, K.; Wright, G.; Junop, M.

Deposited on : 2006-08-17

Resolution : 1.95 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

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)

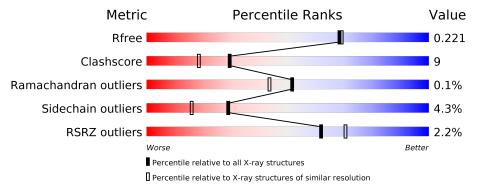
Validation Pipeline (wwPDB-VP) : 2.11

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 1.95 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 ch	ain	
1	A	212	62%	25%	• • 9%
1	В	212	58%	21% • •	17%
1	С	212	65%	21%	• 9%
1	D	212	62%	19% •	16%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6254 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 Phosphoheptose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	192	Total	С	N	О	S	0	0	0
1	A	192	1461	914	261	278	8	0	U	U
1	B	177	Total	С	N	О	S	0	0	0
1	Б	111	1351	846	243	255	7	0	U	, 0
1	С	192	Total	С	N	О	S	0	0	0
1		192	1461	914	261	278	8	0	U	U
1	1 D	178	Total	С	N	О	S	0	0	0
1		110	1357	849	244	257	7		0	

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P63224
A	-18	GLY	_	EXPRESSION TAG	UNP P63224
A	-17	SER	-	EXPRESSION TAG	UNP P63224
A	-16	SER	-	EXPRESSION TAG	UNP P63224
A	-15	HIS	-	EXPRESSION TAG	UNP P63224
A	-14	HIS	-	EXPRESSION TAG	UNP P63224
A	-13	HIS	-	EXPRESSION TAG	UNP P63224
A	-12	HIS	-	EXPRESSION TAG	UNP P63224
A	-11	HIS	_	EXPRESSION TAG	UNP P63224
A	-10	HIS	-	EXPRESSION TAG	UNP P63224
A	-9	SER	-	EXPRESSION TAG	UNP P63224
A	-8	SER	-	EXPRESSION TAG	UNP P63224
A	-7	GLY	-	EXPRESSION TAG	UNP P63224
A	-6	LEU	-	EXPRESSION TAG	UNP P63224
A	-5	VAL	-	EXPRESSION TAG	UNP P63224
A	-4	PRO	_	EXPRESSION TAG	UNP P63224
A	-3	ARG	=	EXPRESSION TAG	UNP P63224
A	-2	GLY	=	EXPRESSION TAG	UNP P63224
A	-1	SER	=	EXPRESSION TAG	UNP P63224
A	0	HIS	-	EXPRESSION TAG	UNP P63224
В	-19	MET	-	EXPRESSION TAG	UNP P63224

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-18	GLY	_	EXPRESSION TAG	UNP P63224
В	-17	SER	-	EXPRESSION TAG	UNP P63224
В	-16	SER	-	EXPRESSION TAG	UNP P63224
В	-15	HIS	-	EXPRESSION TAG	UNP P63224
В	-14	HIS	-	EXPRESSION TAG	UNP P63224
В	-13	HIS	_	EXPRESSION TAG	UNP P63224
В	-12	HIS	_	EXPRESSION TAG	UNP P63224
В	-11	HIS	-	EXPRESSION TAG	UNP P63224
В	-10	HIS	_	EXPRESSION TAG	UNP P63224
В	-9	SER	_	EXPRESSION TAG	UNP P63224
В	-8	SER	-	EXPRESSION TAG	UNP P63224
В	-7	GLY	-	EXPRESSION TAG	UNP P63224
В	-6	LEU	-	EXPRESSION TAG	UNP P63224
В	-5	VAL	_	EXPRESSION TAG	UNP P63224
В	-4	PRO	-	EXPRESSION TAG	UNP P63224
В	-3	ARG	_	EXPRESSION TAG	UNP P63224
В	-2	GLY	-	EXPRESSION TAG	UNP P63224
В	-1	SER	-	EXPRESSION TAG	UNP P63224
В	0	HIS	-	EXPRESSION TAG	UNP P63224
С	-19	MET	-	EXPRESSION TAG	UNP P63224
С	-18	GLY	-	EXPRESSION TAG	UNP P63224
С	-17	SER	-	EXPRESSION TAG	UNP P63224
С	-16	SER	-	EXPRESSION TAG	UNP P63224
С	-15	HIS	-	EXPRESSION TAG	UNP P63224
С	-14	HIS	_	EXPRESSION TAG	UNP P63224
С	-13	HIS	-	EXPRESSION TAG	UNP P63224
С	-12	HIS	-	EXPRESSION TAG	UNP P63224
С	-11	HIS	-	EXPRESSION TAG	UNP P63224
С	-10	HIS	_	EXPRESSION TAG	UNP P63224
С	-9	SER	_	EXPRESSION TAG	UNP P63224
С	-8	SER	_	EXPRESSION TAG	UNP P63224
С	-7	GLY	_	EXPRESSION TAG	UNP P63224
С	-6	LEU	_	EXPRESSION TAG	UNP P63224
С	-5	VAL	_	EXPRESSION TAG	UNP P63224
С	-4	PRO	_	EXPRESSION TAG	UNP P63224
С	-3	ARG	-	EXPRESSION TAG	UNP P63224
С	-2	GLY	-	EXPRESSION TAG	UNP P63224
С	-1	SER	-	EXPRESSION TAG	UNP P63224
С	0	HIS	-	EXPRESSION TAG	UNP P63224
D	-19	MET	-	EXPRESSION TAG	UNP P63224
D	-18	GLY	-	EXPRESSION TAG	UNP P63224
D	-17	SER	-	EXPRESSION TAG	UNP P63224

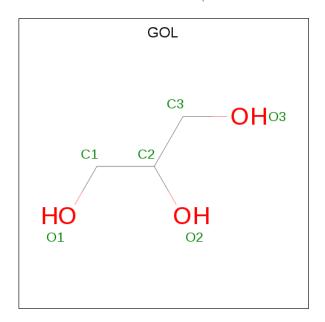
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP P63224
D	-15	HIS	-	EXPRESSION TAG	UNP P63224
D	-14	HIS	-	EXPRESSION TAG	UNP P63224
D	-13	HIS	-	EXPRESSION TAG	UNP P63224
D	-12	HIS	-	EXPRESSION TAG	UNP P63224
D	-11	HIS	-	EXPRESSION TAG	UNP P63224
D	-10	HIS	-	EXPRESSION TAG	UNP P63224
D	-9	SER	-	EXPRESSION TAG	UNP P63224
D	-8	SER	-	EXPRESSION TAG	UNP P63224
D	-7	GLY	-	EXPRESSION TAG	UNP P63224
D	-6	LEU	-	EXPRESSION TAG	UNP P63224
D	-5	VAL	-	EXPRESSION TAG	UNP P63224
D	-4	PRO	-	EXPRESSION TAG	UNP P63224
D	-3	ARG	-	EXPRESSION TAG	UNP P63224
D	-2	GLY	-	EXPRESSION TAG	UNP P63224
D	-1	SER	=	EXPRESSION TAG	UNP P63224
D	0	HIS	-	EXPRESSION TAG	UNP P63224

 \bullet Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 6 3 3	0	0

• Molecule 3 is water.



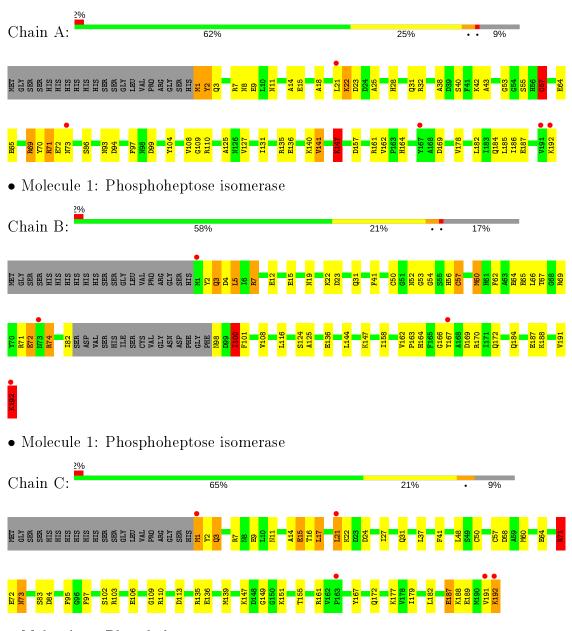
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	167	Total O 167 167	0	0
3	В	142	Total O 142 142	0	0
3	С	150	Total O 150 150	0	0
3	D	159	Total O 159 159	0	0



3 Residue-property plots (i)

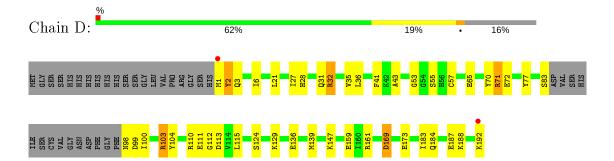
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Phosphoheptose isomerase



• Molecule 1: Phosphoheptose isomerase







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	83.93Å 89.61Å 106.91Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 - 1.95	Depositor
Resolution (A)	45.91 - 1.95	EDS
% Data completeness	$100.0 \ (45.90 - 1.95)$	Depositor
(in resolution range)	99.6 (45.91-1.95)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.65 \; ({\rm at} \; 1.95 {\rm \AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.219	Depositor
10, 10 free	0.173 , 0.221	DCC
R_{free} test set	2996 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 51.5	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6254	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: GOL

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	Chain	Bo	nd lengths	Bond angles		
	RMSZ	# Z > 5	RMSZ	# Z >5		
1	A	1.86	$23/1482 \ (1.6\%)$	1.47	$17/1993 \ (0.9\%)$	
1	В	1.82	23/1368 (1.7%)	1.48	16/1837 (0.9%)	
1	С	1.83	$25/1482 \ (1.7\%)$	1.50	17/1993~(0.9%)	
1	D	1.82	22/1374~(1.6%)	1.49	11/1845~(0.6%)	
All	All	1.84	93/5706 (1.6%)	1.49	61/7668 (0.8%)	

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(\text{\AA})$
1	A	25	ALA	CA-CB	9.46	1.72	1.52
1	В	72	GLU	CG-CD	9.45	1.66	1.51
1	D	136	GLU	CD-OE1	9.21	1.35	1.25
1	С	9	GLU	CD-OE2	9.06	1.35	1.25
1	С	149	GLY	N-CA	-8.84	1.32	1.46

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	A	110	ARG	NE-CZ-NH1	-12.39	114.11	120.30
1	A	157	ASP	CB-CG-OD1	-12.18	107.34	118.30
1	D	71	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	A	157	ASP	CB-CG-OD2	11.47	128.63	118.30
1	D	71	ARG	NE-CZ-NH1	11.10	125.85	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	1461	0	1460	38	0
1	В	1351	0	1366	30	0
1	С	1461	0	1460	28	0
1	D	1357	0	1371	30	0
2	D	6	0	8	0	0
3	A	167	0	0	16	0
3	В	142	0	0	10	0
3	С	150	0	0	1	0
3	D	159	0	0	9	0
All	All	6254	0	5665	106	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.

The worst 5 of 106 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:82:ILE:CG1	1:B:82:ILE:CD1	1.79	1.59
3:A:249:HOH:O	1:D:184:GLN:HG3	1.43	1.15
1:D:98:ASN:HB2	3:D:301:HOH:O	1.46	1.13
1:B:98:ASN:HB2	3:B:324:HOH:O	1.46	1.12
1:B:100:ILE:HG12	3:B:322:HOH:O	1.60	1.01

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	Perce	entiles	
1	A	$190/212 \; (90\%)$	184 (97%)	6 (3%)	0	100	100
1	В	173/212 (82%)	171 (99%)	2 (1%)	0	100	100
1	C	$190/212 \; (90\%)$	189 (100%)	1 (0%)	0	100	100
1	D	$174/212 \; (82\%)$	168 (97%)	5 (3%)	1 (1%)	25	14
All	All	727/848 (86%)	712 (98%)	14 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	TYR

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	151/168 (90%)	145 (96%)	6 (4%)	31 19		
1	В	138/168 (82%)	129 (94%)	9 (6%)	17 6		
1	С	151/168 (90%)	144 (95%)	7 (5%)	27 14		
1	D	139/168 (83%)	136 (98%)	3 (2%)	52 44		
All	All	579/672 (86%)	554 (96%)	25 (4%)	29 16		

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	100	ILE
1	В	191	VAL
1	D	100	ILE
1	В	136	GLU
1	В	192	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:



Mol	Chain	Res	Type
1	В	31	GLN
1	В	56	HIS
1	С	164	HIS
1	В	26	ASN
1	D	26	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 carbohydrates 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	${ m Res}$	Link	\mathbf{B}_{0}	ond leng	${ m gths}$	В	ond ang	gles
L	IVIOI	туре	Chain	rtes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	2	GOL	D	196	ı	5,5,5	0.91	0	5,5,5	2.49	3 (60%)

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	GOL	D	196	-	-	2/4/4/4	-



There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	${f Res}$	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	D	196	GOL	O1-C1-C2	-3.60	92.96	110.20
2	D	196	GOL	O2-C2-C1	3.35	123.86	109.12
2	D	196	GOL	O2-C2-C3	2.52	120.24	109.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	196	GOL	O2-C2-C3-O3
2	D	196	GOL	O1-C1-C2-O2

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 (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^{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 $>$	$\#\mathrm{RSRZ}{>}2$		$\mathrm{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	$192/212 \; (90\%)$	-0.24	5 (2%) 56	65	26, 38, 62, 102	0
1	В	177/212 (83%)	-0.25	4 (2%) 60	69	27, 36, 62, 92	0
1	С	192/212 (90%)	-0.12	5 (2%) 56	65	24, 34, 63, 96	0
1	D	178/212 (83%)	-0.22	2 (1%) 80	85	25,33,55,83	0
All	All	739/848 (87%)	-0.21	16 (2%) 62	70	24, 35, 62, 102	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	6.2
1	С	191	VAL	4.3
1	A	191	VAL	4.1
1	С	1	MET	3.4
1	В	167	TYR	3.2

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 carbohydrates 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
2	GOL	D	196	6/6	0.91	0.14	$44,\!51,\!53,\!63$	0

6.5 Other polymers (i)

There are no such residues in this entry.

