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 ⓘ

Jan 23, 2021 – 03:36 PM EST

PDB ID	:	1XEA
Title	:	Crystal structure of a Gfo/Idh/MocA family oxidoreductase from Vibrio cholerae
Authors	:	R Rajashankar, K.; Reynes, J.A.; Kniewel, R.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-09-09
Resolution	:	2.65 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

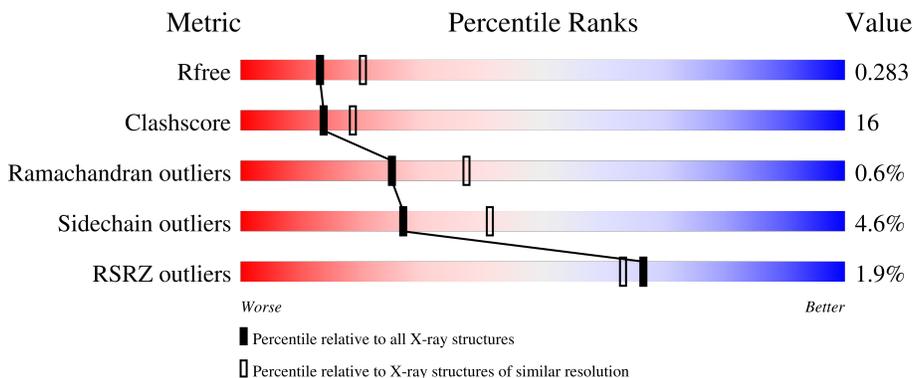|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.65 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		16
Ramachandran outliers		0.6%
Sidechain outliers		4.6%
RSRZ outliers		1.9%

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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	323	2% · 68% · 26% · ·
1	B	323	2% · 67% · 27% · ·
1	C	323	2% · 62% · 32% · ·
1	D	323	2% · 68% · 26% · ·

2　Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10198 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 Oxidoreductase, Gfo/Idh/MocA family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	Se	0	0	0
			2481	1574	439	455	6	7			
1	B	311	Total	C	N	O	S	Se	0	0	0
			2481	1574	439	455	6	7			
1	C	311	Total	C	N	O	S	Se	0	0	0
			2481	1574	439	455	6	7			
1	D	311	Total	C	N	O	S	Se	0	0	0
			2481	1574	439	455	6	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q9KKQ4
A	2	SER	-	cloning artifact	UNP Q9KKQ4
A	3	LEU	-	cloning artifact	UNP Q9KKQ4
A	7	MSE	MET	modified residue	UNP Q9KKQ4
A	68	MSE	MET	modified residue	UNP Q9KKQ4
A	192	MSE	MET	modified residue	UNP Q9KKQ4
A	215	MSE	MET	modified residue	UNP Q9KKQ4
A	245	MSE	MET	modified residue	UNP Q9KKQ4
A	262	MSE	MET	modified residue	UNP Q9KKQ4
A	271	MSE	MET	modified residue	UNP Q9KKQ4
A	314	GLU	-	expression tag	UNP Q9KKQ4
A	315	GLY	-	expression tag	UNP Q9KKQ4
A	316	GLY	-	expression tag	UNP Q9KKQ4
A	317	SER	-	expression tag	UNP Q9KKQ4
A	318	HIS	-	expression tag	UNP Q9KKQ4
A	319	HIS	-	expression tag	UNP Q9KKQ4
A	320	HIS	-	expression tag	UNP Q9KKQ4
A	321	HIS	-	expression tag	UNP Q9KKQ4
A	322	HIS	-	expression tag	UNP Q9KKQ4
A	323	HIS	-	expression tag	UNP Q9KKQ4
B	1	MET	-	cloning artifact	UNP Q9KKQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	cloning artifact	UNP Q9KKQ4
B	3	LEU	-	cloning artifact	UNP Q9KKQ4
B	7	MSE	MET	modified residue	UNP Q9KKQ4
B	68	MSE	MET	modified residue	UNP Q9KKQ4
B	192	MSE	MET	modified residue	UNP Q9KKQ4
B	215	MSE	MET	modified residue	UNP Q9KKQ4
B	245	MSE	MET	modified residue	UNP Q9KKQ4
B	262	MSE	MET	modified residue	UNP Q9KKQ4
B	271	MSE	MET	modified residue	UNP Q9KKQ4
B	314	GLU	-	expression tag	UNP Q9KKQ4
B	315	GLY	-	expression tag	UNP Q9KKQ4
B	316	GLY	-	expression tag	UNP Q9KKQ4
B	317	SER	-	expression tag	UNP Q9KKQ4
B	318	HIS	-	expression tag	UNP Q9KKQ4
B	319	HIS	-	expression tag	UNP Q9KKQ4
B	320	HIS	-	expression tag	UNP Q9KKQ4
B	321	HIS	-	expression tag	UNP Q9KKQ4
B	322	HIS	-	expression tag	UNP Q9KKQ4
B	323	HIS	-	expression tag	UNP Q9KKQ4
C	1	MET	-	cloning artifact	UNP Q9KKQ4
C	2	SER	-	cloning artifact	UNP Q9KKQ4
C	3	LEU	-	cloning artifact	UNP Q9KKQ4
C	7	MSE	MET	modified residue	UNP Q9KKQ4
C	68	MSE	MET	modified residue	UNP Q9KKQ4
C	192	MSE	MET	modified residue	UNP Q9KKQ4
C	215	MSE	MET	modified residue	UNP Q9KKQ4
C	245	MSE	MET	modified residue	UNP Q9KKQ4
C	262	MSE	MET	modified residue	UNP Q9KKQ4
C	271	MSE	MET	modified residue	UNP Q9KKQ4
C	314	GLU	-	expression tag	UNP Q9KKQ4
C	315	GLY	-	expression tag	UNP Q9KKQ4
C	316	GLY	-	expression tag	UNP Q9KKQ4
C	317	SER	-	expression tag	UNP Q9KKQ4
C	318	HIS	-	expression tag	UNP Q9KKQ4
C	319	HIS	-	expression tag	UNP Q9KKQ4
C	320	HIS	-	expression tag	UNP Q9KKQ4
C	321	HIS	-	expression tag	UNP Q9KKQ4
C	322	HIS	-	expression tag	UNP Q9KKQ4
C	323	HIS	-	expression tag	UNP Q9KKQ4
D	1	MET	-	cloning artifact	UNP Q9KKQ4
D	2	SER	-	cloning artifact	UNP Q9KKQ4
D	3	LEU	-	cloning artifact	UNP Q9KKQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	7	MSE	MET	modified residue	UNP Q9KKQ4
D	68	MSE	MET	modified residue	UNP Q9KKQ4
D	192	MSE	MET	modified residue	UNP Q9KKQ4
D	215	MSE	MET	modified residue	UNP Q9KKQ4
D	245	MSE	MET	modified residue	UNP Q9KKQ4
D	262	MSE	MET	modified residue	UNP Q9KKQ4
D	271	MSE	MET	modified residue	UNP Q9KKQ4
D	314	GLU	-	expression tag	UNP Q9KKQ4
D	315	GLY	-	expression tag	UNP Q9KKQ4
D	316	GLY	-	expression tag	UNP Q9KKQ4
D	317	SER	-	expression tag	UNP Q9KKQ4
D	318	HIS	-	expression tag	UNP Q9KKQ4
D	319	HIS	-	expression tag	UNP Q9KKQ4
D	320	HIS	-	expression tag	UNP Q9KKQ4
D	321	HIS	-	expression tag	UNP Q9KKQ4
D	322	HIS	-	expression tag	UNP Q9KKQ4
D	323	HIS	-	expression tag	UNP Q9KKQ4

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ni 1	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total 69	O 69	0	0
3	B	66	Total 66	O 66	0	0
3	C	68	Total 68	O 68	0	0
3	D	70	Total 70	O 70	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.
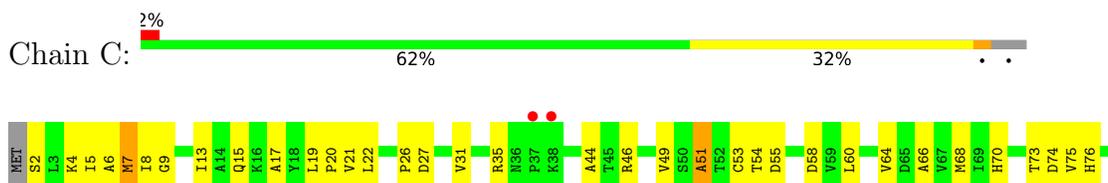
- Molecule 1: Oxidoreductase, Gfo/Idh/MocA family
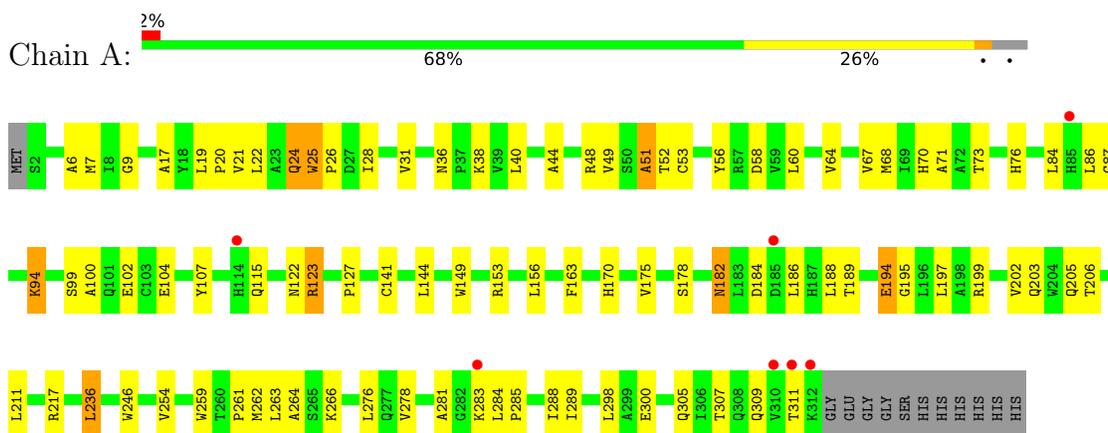
Chain A:

- Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain B:

- Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain C:

• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain D:
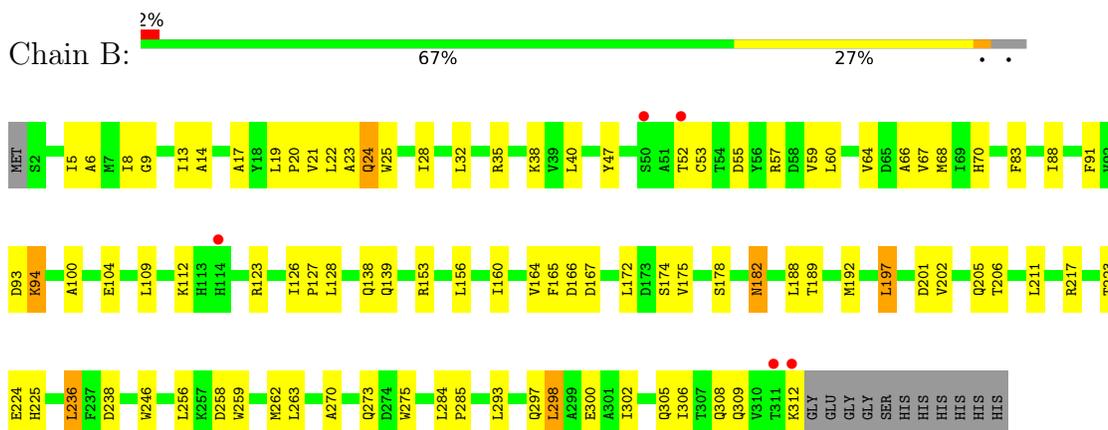
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.53Å 112.83Å 177.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.65 19.99 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.2 (19.99-2.65) 98.1 (19.99-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.67Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.271 0.240 , 0.283	Depositor DCC
R_{free} test set	4434 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10198	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1482e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: NI

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	0.40	0/2533	0.57	0/3434
1	B	0.38	0/2533	0.57	0/3434
1	C	0.40	0/2533	0.58	0/3434
1	D	0.40	0/2533	0.59	0/3434
All	All	0.39	0/10132	0.58	0/13736

There are no bond length outliers.

There are no bond angle outliers.

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	2481	0	2437	75	0
1	B	2481	0	2437	78	0
1	C	2481	0	2437	99	0
1	D	2481	0	2437	81	0
2	A	1	0	0	0	0
3	A	69	0	0	1	0
3	B	66	0	0	2	0
3	C	68	0	0	2	0
3	D	70	0	0	2	0
All	All	10198	0	9748	313	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 16.

The worst 5 of 313 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:D:215:MSE:HE3	1:D:217:ARG:HD3	1.16	1.10
1:C:222:THR:H	1:D:249:ASN:HD21	1.15	0.94
1:D:198:ALA:HB1	1:D:218:GLN:HG3	1.48	0.93
1:D:215:MSE:HE3	1:D:217:ARG:CD	2.00	0.92
1:C:7:MSE:HE2	1:C:19:LEU:HD13	1.52	0.90

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	309/323 (96%)	276 (89%)	30 (10%)	3 (1%)	15	23
1	B	309/323 (96%)	274 (89%)	34 (11%)	1 (0%)	41	56
1	C	309/323 (96%)	281 (91%)	26 (8%)	2 (1%)	25	37
1	D	309/323 (96%)	286 (93%)	22 (7%)	1 (0%)	41	56
All	All	1236/1292 (96%)	1117 (90%)	112 (9%)	7 (1%)	25	37

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	ALA
1	A	51	ALA
1	A	71	ALA
1	B	35	ARG
1	D	56	TYR

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	266/268 (99%)	253 (95%)	13 (5%)	25	38
1	B	266/268 (99%)	255 (96%)	11 (4%)	30	46
1	C	266/268 (99%)	256 (96%)	10 (4%)	33	49
1	D	266/268 (99%)	251 (94%)	15 (6%)	21	33
All	All	1064/1072 (99%)	1015 (95%)	49 (5%)	27	41

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	236	LEU
1	C	182	ASN
1	D	249	ASN
1	C	7	MSE
1	C	184	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	GLN
1	C	203	GLN
1	D	273	GLN
1	C	76	HIS
1	C	131	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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, 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(Å²)	Q<0.9
1	A	304/323 (94%)	-0.14	7 (2%)	60	56	26, 50, 72, 85	0
1	B	304/323 (94%)	-0.06	5 (1%)	72	69	25, 55, 78, 86	0
1	C	304/323 (94%)	-0.21	5 (1%)	72	69	27, 48, 71, 82	0
1	D	304/323 (94%)	-0.25	6 (1%)	65	60	23, 45, 63, 71	0
All	All	1216/1292 (94%)	-0.17	23 (1%)	66	63	23, 48, 73, 86	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	LYS	3.1
1	C	283	LYS	3.0
1	B	52	THR	2.9
1	A	311	THR	2.8
1	A	114	HIS	2.7

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	NI	A	1001	1/1	0.91	0.07	57,57,57,57	1

6.5   Other polymers ⓘ

There are no such residues in this entry.