

wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 12:32 pm GMT

ViFe- hydro-

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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.08 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.



Matria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	А	264	89%	9%	
1	В	264	3% 91%	8%	·
1	С	264	91%	8%	•
2	Q	549	91%	8%	·
2	R	549	% 93%	6%	5 •

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Mol	Chain	Length	Quality of chain		
			5%		
2	S	549	91%	8%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	Q	1564	-	-	Х	-



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 20352 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.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace		
1	Δ	262	Total	С	Ν	0	\mathbf{S}	0	0	0	
	A	262	1973	1256	330	372	15	0	0	U	
1	D	262	Total	С	Ν	0	\mathbf{S}	0	2	0	
	D	202	1980	1260	330	375	15	0	2		
1	C	260	Total	С	Ν	0	S	0	1	0	
		260	1964	1251	328	370	15	U		U	

• Molecule 1 is a protein called PERIPLASMIC [NIFE] HYDROGENASE SMALL SUBUNIT.

• Molecule 2 is a protein called PERIPLASMIC [NIFE] HYDROGENASE LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	2 Q 544	544	Total	С	Ν	Ο	S	0	0	0
		044	4204	2680	728	774	22	0	9	0
0	D	545	Total	С	Ν	0	S	0	2	0
	π	040	4181	2664	724	771	22	0	5	
0	C	544	Total	С	Ν	0	S	0	1	0
	2 5	544	4169	2654	724	769	22	0	L	0

• Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	TotalFeS844	0	0
3	А	1	TotalFeS844	0	0
3	В	1	TotalFeS844	0	0
3	В	1	TotalFeS844	0	0
3	С	1	TotalFeS844	0	0
3	С	1	TotalFeS844	0	0

• Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	TotalFeS734	0	0
4	В	1	TotalFeS734	0	0
4	С	1	TotalFeS734	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	А	1	Total 6	C 3	0 3	0	0

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Total

С

3 3

Ο

 \mathbf{S}

• Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Chain Residues AltConf ZeroOcc Mol Atoms С Total А С Total А Total С Ο Q Total С Q Total С Ο Q С Total Q Total С R Total С R Total С R С Total R С Total R Total С Ο R

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	0 1	1	Total	С	Fe	Ν	Ο	0	0
0	Q	1	7	3	1	2	1	0	0
6	В	1	Total	С	Fe	Ν	Ο	0	0
0	п	1	7	3	1	2	1	0	0
6	S	1	Total	С	Fe	Ν	Ο	0	0
0	2	1	7	3	1	2	1	0	0

• Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Q	1	Total Ni 1 1	0	0
7	R	1	Total Ni 1 1	0	0
7	S	1	Total Ni 1 1	0	0

• Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Q	1	Total Mg 1 1	0	0
8	R	1	Total Mg 1 1	0	0
8	S	1	Total Mg 1 1	0	0



• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	310	Total O 310 310	0	0
9	В	191	Total O 191 191	0	0
9	С	216	Total O 216 216	0	0
9	Q	405	Total O 405 405	0	0
9	R	342	Total O 342 342	0	0
9	S	237	Total O 237 237	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: PERIPLASMIC [NIFE] HYDROGENASE SMALL SUBUNIT





• Molecule 2: PERIPLASMIC [NIFE] HYDROGENASE LARGE SUBUNIT





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	64.77Å 100.40Å 183.43Å	Deperitor
a, b, c, α , β , γ	90.00° 91.55° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	21.98 - 2.08	Depositor
Resolution (A)	21.98 - 2.08	EDS
% Data completeness	87.6 (21.98-2.08)	Depositor
(in resolution range)	87.7 (21.98-2.08)	EDS
R_{merge}	0.04	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$6.18 (at 2.08 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
P. P.	0.195 , 0.235	Depositor
Π, Π_{free}	0.195 , 0.235	DCC
R_{free} test set	6255 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	18.8	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 56.5	EDS
L-test for twinning ²	$< L >=0.39, < L^2>=0.21$	Xtriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20352	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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, NI, SF4, MG, FCO, F3S, CSO

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).

Mal	Chain	Bo	ond lengths	B	ond angles
10101	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.74	4/2027~(0.2%)	0.75	4/2759~(0.1%)
1	В	0.53	1/2043~(0.0%)	0.61	0/2781
1	С	0.68	8/2023~(0.4%)	0.66	2/2754~(0.1%)
2	Q	0.58	2/4334~(0.0%)	0.68	3/5881~(0.1%)
2	R	0.50	2/4292~(0.0%)	0.64	3/5825~(0.1%)
2	S	0.43	1/4271~(0.0%)	0.60	3/5796~(0.1%)
All	All	0.56	18/18990~(0.1%)	0.65	15/25796~(0.1%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	R	517	GLU	CD-OE2	-10.55	1.14	1.25
1	С	261	TYR	CE1-CZ	-10.53	1.24	1.38
2	Q	464	GLU	CD-OE1	-9.32	1.15	1.25
1	С	261	TYR	CG-CD2	-9.06	1.27	1.39
1	С	261	TYR	CG-CD1	-8.65	1.27	1.39

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	R	517	GLU	OE1-CD-OE2	-9.88	111.45	123.30
2	Q	464	GLU	OE1-CD-OE2	-7.94	113.77	123.30
2	S	161	LYS	CD-CE-NZ	7.87	129.79	111.70
1	А	203	ASP	CB-CG-OD2	7.55	125.09	118.30
1	С	215	GLU	OE1-CD-OE2	-7.03	114.86	123.30

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	А	1973	0	1911	13	0
1	В	1980	0	1918	21	0
1	С	1964	0	1906	19	0
2	Q	4204	0	4192	31	0
2	R	4181	0	4154	24	0
2	S	4169	0	4140	28	0
3	А	16	0	0	0	0
3	В	16	0	0	0	0
3	С	16	0	0	0	0
4	А	7	0	0	0	0
4	В	7	0	0	0	0
4	С	7	0	0	0	0
5	А	18	0	24	3	0
5	Q	24	0	32	5	0
5	R	36	0	48	3	0
5	S	6	0	8	0	0
6	Q	7	0	0	1	0
6	R	7	0	0	0	0
6	S	7	0	0	1	0
7	Q	1	0	0	0	0
7	R	1	0	0	0	0
7	S	1	0	0	0	0
8	Q	1	0	0	0	0
8	R	1	0	0	0	0
8	S	1	0	0	0	0
9	А	310	0	0	4	0
9	В	191	0	0	2	0
9	С	216	0	0	5	0
9	Q	405	0	0	2	0
9	R	342	0	0	4	0
9	S	237	0	0	5	0
All	All	20352	0	18333	124	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 124 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:B:202:PHE:CE2	2:R:233:VAL:HG11	1.83	1.13
1:B:202:PHE:CE1	1:B:216:LEU:HD13	1.87	1.09
1:B:202:PHE:CD2	2:R:233:VAL:HG11	1.95	1.00
9:C:2216:HOH:O	2:Q:189:LYS:HE3	1.73	0.88
2:Q:337:LYS:HE2	5:Q:1564:GOL:H2	1.56	0.85

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	ntiles
1	А	260/264~(98%)	254 (98%)	6 (2%)	0	100	100
1	В	262/264~(99%)	254 (97%)	8 (3%)	0	100	100
1	С	259/264~(98%)	251 (97%)	8 (3%)	0	100	100
2	Q	550/549~(100%)	533~(97%)	17 (3%)	0	100	100
2	R	545/549~(99%)	534 (98%)	11 (2%)	0	100	100
2	S	542/549~(99%)	524 (97%)	18 (3%)	0	100	100
All	All	2418/2439~(99%)	2350 (97%)	68 (3%)	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	Perce	ntiles
1	А	208/210~(99%)	206~(99%)	2(1%)	76	81
1	В	210/210~(100%)	209 (100%)	1 (0%)	88	92
1	С	208/210~(99%)	208 (100%)	0	100	100
2	Q	443/438 (101%)	438 (99%)	5 (1%)	73	78
2	R	437/438~(100%)	432~(99%)	5(1%)	73	78
2	S	435/438~(99%)	429~(99%)	6 (1%)	67	72
All	All	1941/1944 (100%)	1922 (99%)	19 (1%)	76	81

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
2	S	397	GLN
2	S	416	THR
2	S	473	ASP
2	S	408	LEU
2	R	92	LYS

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

Mol	Chain	Res	Type
1	А	14	ASN
1	В	14	ASN
1	В	61	HIS
1	С	14	ASN
1	С	172	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)

3 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



Mal	Mol Type Chain B	Dec	Tink	Bond lengths			Bond angles			
Wor Type Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
2	CSO	Q	543	7,2	3,6,7	0.54	0	$0,\!6,\!8$	-	-
2	CSO	S	543	7,2	3,6,7	0.83	0	$0,\!6,\!8$	-	-
2	CSO	R	543	7,2	3,6,7	0.66	0	$0,\!6,\!8$	-	-

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).

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	CSO	Q	543	7,2	-	1/1/5/7	-
2	CSO	S	543	7,2	-	1/1/5/7	-
2	CSO	R	543	7,2	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	543	CSO	N-CA-CB-SG
2	R	543	CSO	N-CA-CB-SG
2	S	543	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 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).

Mal	Turne	Chain	Dec	Timle	В	Bond lengths		Bond angles		
	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	F3S	A	1266	1	0,9,9	-	-	-		
4	F3S	В	1266	1	0,9,9	-	-	-		
5	GOL	R	1565	-	$5,\!5,\!5$	0.32	0	$5,\!5,\!5$	0.20	0
6	FCO	Q	1550	7,2	0,6,6	-	-	-		
5	GOL	R	1564	-	$5,\!5,\!5$	0.33	0	$5,\!5,\!5$	0.18	0
5	GOL	R	1563	-	$5,\!5,\!5$	0.26	0	$5,\!5,\!5$	0.43	0
3	SF4	С	1265	1	0,12,12	-	-	-		,
4	F3S	С	1266	1	0,9,9	-	-	-		
5	GOL	S	1561	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.24	0
5	GOL	Q	1563	-	$5,\!5,\!5$	0.27	0	$5,\!5,\!5$	0.26	0
3	SF4	С	1267	1	0,12,12	-	-	-		
5	GOL	R	1562	-	$5,\!5,\!5$	0.26	0	$5,\!5,\!5$	0.18	0
5	GOL	R	1566	_	$5,\!5,\!5$	0.36	0	$5,\!5,\!5$	0.27	0
3	SF4	А	1265	1	0,12,12	-	-	-		,
5	GOL	Q	1562	-	$5,\!5,\!5$	0.20	0	$5,\!5,\!5$	0.30	0
5	GOL	Q	1561	-	$5,\!5,\!5$	0.26	0	$5,\!5,\!5$	0.18	0
5	GOL	А	1271	-	$5,\!5,\!5$	0.30	0	$5,\!5,\!5$	0.55	0
3	SF4	В	1265	1	0,12,12	-	-	-		,
5	GOL	А	1273	-	$5,\!5,\!5$	0.39	0	$5,\!5,\!5$	0.54	0
6	FCO	S	1550	7,2	0,6,6	-	-	-		,
3	SF4	А	1267	1	0,12,12	-	-	-		
3	SF4	В	1267	1	0,12,12	-	-	-		
5	GOL	Q	1564	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.46	0
6	FCO	R	1550	7,2	0,6,6	-	-	-		
5	GOL	R	1561	-	$5,\!5,\!5$	0.31	0	$5,\!5,\!5$	0.61	0
5	GOL	А	1272	-	$5,\!5,\!5$	0.33	0	$5,\!5,\!5$	0.42	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
5	GOL	R	1565	-	-	4/4/4/4	-
4	F3S	А	1266	1	-	-	0/3/3/3
4	F3S	В	1266	1	-	-	0/3/3/3
5	GOL	R	1564	-	-	2/4/4/4	-



40LW	4UE	W
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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	R	1563	-	-	0/4/4/4	-
3	SF4	С	1265	1	-	-	0/6/5/5
5	GOL	S	1561	-	-	0/4/4/4	-
4	F3S	С	1266	1	-	-	0/3/3/3
5	GOL	Q	1563	-	-	0/4/4/4	-
3	SF4	С	1267	1	-	-	0/6/5/5
5	GOL	R	1562	-	-	4/4/4/4	-
5	GOL	R	1566	-	-	4/4/4/4	-
5	GOL	Q	1562	-	-	0/4/4/4	-
3	SF4	А	1265	1	-	-	0/6/5/5
5	GOL	Q	1561	-	-	0/4/4/4	-
5	GOL	А	1273	-	-	2/4/4/4	-
5	GOL	А	1271	-	-	3/4/4/4	-
3	SF4	В	1265	1	-	-	0/6/5/5
3	SF4	А	1267	1	-	-	0/6/5/5
3	SF4	В	1267	1	-	-	0/6/5/5
5	GOL	Q	1564	-	-	2/4/4/4	-
5	GOL	R	1561	-	-	1/4/4/4	-
5	GOL	А	1272	-	-	2/4/4/4	-

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There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	1271	GOL	C1-C2-C3-O3
5	R	1562	GOL	O1-C1-C2-C3
5	R	1566	GOL	O1-C1-C2-O2
5	R	1566	GOL	O1-C1-C2-C3
5	R	1566	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	1550	FCO	1	0
5	R	1564	GOL	1	0
5	Q	1563	GOL	1	0

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	0	-	1 0		
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	1562	GOL	2	0
5	А	1273	GOL	3	0
6	S	1550	FCO	1	0
5	Q	1564	GOL	4	0

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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 $>$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	262/264~(99%)	-0.56	0 100 100	9, 17, 27, 46	4 (1%)
1	В	262/264~(99%)	0.17	9 (3%) 45 50	21, 36, 57, 71	6(2%)
1	С	260/264~(98%)	-0.05	0 100 100	19, 33, 56, 70	4 (1%)
2	Q	543/549~(98%)	-0.52	0 100 100	9, 19, 33, 42	7(1%)
2	R	544/549~(99%)	-0.19	4 (0%) 87 89	16, 29, 47, 65	6 (1%)
2	S	543/549~(98%)	0.41	25 (4%) 32 36	20, 48, 77, 90	7(1%)
All	All	2414/2439 (98%)	-0.12	38 (1%) 72 75	9, 29, 63, 90	34 (1%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	264	GLY	5.5
2	S	400	PHE	4.2
2	S	280	TRP	3.9
2	S	160	LEU	3.9
2	S	134	LEU	3.6

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, 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	CSO	S	543	7/8	0.97	0.09	29,31,32,33	1
2	CSO	R	543	7/8	0.99	0.06	18,18,19,19	1
2	CSO	Q	543	7/8	0.99	0.06	9,9,10,10	1



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	$B-factors(A^2)$	Q<0.9
5	GOL	R	1566	6/6	0.67	0.25	55,60,61,62	0
5	GOL	R	1562	6/6	0.83	0.19	49,50,52,53	0
5	GOL	Q	1563	6/6	0.83	0.20	43,49,53,53	0
5	GOL	Q	1564	6/6	0.85	0.20	36,38,41,46	0
5	GOL	S	1561	6/6	0.85	0.15	34,40,41,42	0
5	GOL	R	1563	6/6	0.89	0.15	34,36,38,39	0
5	GOL	А	1273	6/6	0.91	0.17	43,43,46,47	0
5	GOL	R	1564	6/6	0.91	0.20	40,43,47,53	0
5	GOL	R	1565	6/6	0.93	0.13	40,41,42,42	0
5	GOL	Q	1561	6/6	0.94	0.16	35,36,38,39	0
5	GOL	А	1272	6/6	0.95	0.16	39,39,42,46	0
8	MG	S	1553	1/1	0.95	0.05	34,34,34,34	0
3	SF4	В	1265	8/8	0.96	0.07	45,47,48,50	0
5	GOL	R	1561	6/6	0.96	0.08	28,29,30,30	0
5	GOL	А	1271	6/6	0.96	0.11	25,30,32,36	0
8	MG	R	1553	1/1	0.97	0.03	24,24,24,24	0
5	GOL	Q	1562	6/6	0.98	0.11	20,22,23,25	0
3	SF4	В	1267	8/8	0.98	0.06	24,25,26,26	0
4	F3S	В	1266	7/7	0.99	0.04	32,32,34,34	0
4	F3S	С	1266	7/7	0.99	0.05	20,21,21,22	0
3	SF4	А	1267	8/8	0.99	0.07	8,8,9,9	0
3	SF4	С	1265	8/8	0.99	0.07	19,21,21,22	0
6	FCO	R	1550	7/7	0.99	0.08	19,20,20,21	0
6	FCO	S	1550	7/7	0.99	0.12	29,30,31,32	0
7	NI	S	1551	1/1	0.99	0.08	27,27,27,27	0
8	MG	Q	1553	1/1	0.99	0.06	9,9,9,9	0
3	SF4	С	1267	8/8	0.99	0.07	23,23,24,25	0
4	F3S	А	1266	7/7	0.99	0.06	9,10,10,10	0
3	SF4	А	1265	8/8	1.00	0.06	13,14,15,15	0
6	FCO	Q	1550	7/7	1.00	0.07	9,9,9,9	0
7	NI	Q	1551	1/1	1.00	0.07	10,10,10,10	0
7	NI	R	1551	1/1	1.00	0.06	20,20,20,20	0



6.5 Other polymers (i)

There are no such residues in this entry.

