

Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2025 – 02:38 pm GMT

:	9ER7
:	Hydrogenase-1 Ni-SCO state
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:	2024-03-22
:	1.40 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 (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	:	3.0
buster-report	:	1.1.7(2018)
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)	:	2.41.5

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 1.40 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.



Motria	Whole archive	Similar resolution
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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	S	279	^{2%} 87%	6%	6%
1	Т	279	% 90%	•	6%
2	L	582	^{2%} 94%		6% •
2	М	582	% 94%		5%•

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
11	CMO	L	605	-	-	Х	-
11	CMO	М	604	-	-	Х	Х



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 14827 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 Hydrogenase-1 small chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	S	263	Total 2054	C 1305	N 353	O 376	S 20	0	4	0
1	Т	263	Total 2082	C 1322	N 355	0 384	S 21	0	8	0

Chain	Residue	Modelled	Actual	Comment	Reference
S	272	ARG	-	expression tag	UNP P69739
S	273	SER	-	expression tag	UNP P69739
S	274	HIS	-	expression tag	UNP P69739
S	275	HIS	-	expression tag	UNP P69739
S	276	HIS	-	expression tag	UNP P69739
S	277	HIS	-	expression tag	UNP P69739
S	278	HIS	-	expression tag	UNP P69739
S	279	HIS	-	expression tag	UNP P69739
Т	272	ARG	-	expression tag	UNP P69739
Т	273	SER	-	expression tag	UNP P69739
Т	274	HIS	-	expression tag	UNP P69739
Т	275	HIS	-	expression tag	UNP P69739
Т	276	HIS	-	expression tag	UNP P69739
Т	277	HIS	-	expression tag	UNP P69739
Т	278	HIS	-	expression tag	UNP P69739
Т	279	HIS	_	expression tag	UNP P69739

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total 4625	C 2935	N 812	O 850	S 28	0	13	0
2	М	581	Total 4630	C 2937	N 810	O 856	S 27	0	13	0



 $\bullet\,$ Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	S	1	TotalFeS844	0	0
3	Т	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	S	1	Total 7	${ m Fe} \ 3$	${S \atop 4}$	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	Т	1	Total 7	Fe 3	$\frac{S}{4}$	0	0

• Molecule 5 is FE4-S3 CLUSTER (three-letter code: SF3) (formula: Fe_4S_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	1	TotalFeS743	0	0
5	Т	1	TotalFeS743	0	0

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	S	2	Total Cl 2 2	0	0
6	Т	2	Total Cl 2 2	0	0





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	Т	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
7	М	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 8 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
8	L	1	Total	С	Fe	Ν	0	0	0
0		T	7	3	1	2	1	0	0
8	М	1	Total	С	Fe	Ν	Ο	0	0
0	111	T	7	3	1	2	1	0	0

• Molecule 9 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total Ni 1 1	0	0
9	М	1	Total Ni 1 1	0	0

• Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total Mg 1 1	0	0
10	М	1	Total Mg 1 1	0	0

• Molecule 11 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 2 1 1 \end{array}$	0	0
11	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 2 & 1 & 1 \end{array}$	0	0

• Molecule 12 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1, 3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total 8	С 4	N 1	O 3	0	0

• Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	S	204	Total O 204 204	0	0
13	L	443	Total O 443 443	0	0
13	Т	199	Total O 199 199	0	0
13	М	497	Total O 497 497	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: Hydrogenase-1 small chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	93.79Å 96.01Å 182.79Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	66.20 - 1.40	Depositor
Resolution (A)	$66.20 \ - \ 1.40$	EDS
% Data completeness	99.9 (66.20-1.40)	Depositor
(in resolution range)	99.9 (66.20-1.40)	EDS
R _{merge}	0.27	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.17 (at 1.40 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
D D.	0.169 , 0.189	Depositor
Π, Π_{free}	0.173 , 0.195	DCC
R_{free} test set	16216 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	16.0	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.35 , 31.9	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14827	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.83% 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: SF3, SF4, F3S, SO4, TRS, CL, FCO, NI, MG, CMO

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		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	S	0.50	0/2118	0.86	2/2875~(0.1%)	
1	Т	0.52	0/2152	0.89	3/2920~(0.1%)	
2	L	0.48	0/4777	0.85	8/6496~(0.1%)	
2	М	0.50	0/4777	0.86	10/6500~(0.2%)	
All	All	0.50	0/13824	0.86	23/18791~(0.1%)	

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	S	0	4
1	Т	0	3
2	L	0	3
2	М	0	3
All	All	0	13

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Т	234	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	Т	234	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	S	193	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	S	193	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	М	169	ARG	CG-CD-NE	6.93	126.35	111.80
2	М	275	MET	CG-SD-CE	-6.66	89.54	100.20
1	Т	177	ARG	NE-CZ-NH1	6.59	123.59	120.30
2	М	434	MET	CG-SD-CE	6.49	110.59	100.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	М	63	ARG	CA-CB-CG	-6.49	99.12	113.40
2	М	363	ARG	NE-CZ-NH2	5.92	123.26	120.30
2	М	89	TYR	CB-CG-CD1	5.88	124.53	121.00
2	L	457	HIS	CB-CA-C	5.61	121.63	110.40
2	L	17[A]	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	L	17[B]	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	L	500	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	L	89	TYR	CB-CG-CD1	5.39	124.23	121.00
2	L	519	ARG	NE-CZ-NH1	-5.31	117.64	120.30
2	L	89	TYR	CB-CG-CD2	-5.26	117.84	121.00
2	М	500[A]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	М	500[B]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	М	458	GLU	CG-CD-OE2	-5.21	107.87	118.30
2	М	32	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	L	356	TYR	CB-CA-C	-5.11	100.18	110.40

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There are no chirality outliers.

Mol	Chain	Res	Type	Group
2	L	256[A]	ARG	Sidechain
2	L	256[B]	ARG	Sidechain
2	L	74	ARG	Sidechain
2	М	169	ARG	Sidechain
2	М	256[A]	ARG	Sidechain
2	М	74	ARG	Sidechain
1	S	174	ARG	Sidechain
1	S	26	ARG	Sidechain
1	S	260	ARG	Sidechain
1	S	266	ARG	Sidechain
1	Т	101	ARG	Sidechain
1	Т	234	ARG	Sidechain
1	Т	26	ARG	Sidechain

All (13) planarity outliers are listed below:

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	${ m H}({ m model})$	H(added)	Clashes	Symm-Clashes
1	S	2054	0	2002	9	0
1	Т	2082	0	2025	6	0
2	L	4625	0	4529	26	0
2	М	4630	0	4512	23	0
3	S	8	0	0	0	0
3	Т	8	0	0	0	0
4	S	7	0	0	0	0
4	Т	7	0	0	0	0
5	S	7	0	0	0	0
5	Т	7	0	0	0	0
6	S	2	0	0	0	0
6	Т	2	0	0	0	0
7	L	5	0	0	0	0
7	М	5	0	0	0	0
7	Т	5	0	0	0	0
8	L	7	0	0	0	0
8	М	7	0	0	0	0
9	L	1	0	0	0	0
9	М	1	0	0	0	0
10	L	1	0	0	0	0
10	М	1	0	0	0	0
11	L	2	0	0	5	0
11	М	2	0	0	4	0
12	L	8	0	12	0	0
13	L	443	0	0	6	0
13	М	497	0	0	7	0
13	S	204	0	0	4	0
13	Т	199	0	0	3	0
All	All	14827	0	13080	63	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 2.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:M:269[B]:ASP:OD1	13:M:701:HOH:O	1.89	0.89
2:M:39[A]:ASP:OD2	13:M:702:HOH:O	1.98	0.81
2:M:269[A]:ASP:OD2	13:M:703:HOH:O	2.01	0.77
2:L:509:ARG:NH1	11:L:605:CMO:C	2.53	0.71
1:T:167[A]:ASP:OD1	13:T:501:HOH:O	2.09	0.70
2:M:39[A]:ASP:CG	13:M:702:HOH:O	2.29	0.70



Atom 1	Atom 9	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:M:39[A]:ASP:OD1	13:M:702:HOH:O	2.10	0.70	
2:L:509:ARG:CZ	11:L:605:CMO:C	2.73	0.66	
1:S:6:ARG:NH2	13:S:501:HOH:O	2.29	0.64	
2:L:498:GLU:HG2	2:L:519:ARG:HG3	1.81	0.63	
2:L:275[B]:MET:CE	2:L:456:ALA:HA	2.30	0.62	
2:M:509:ARG:NH1	11:M:604:CMO:C	2.64	0.60	
2:L:509:ARG:CZ	11:L:605:CMO:O	2.50	0.59	
1:S:260:ARG:HG3	13:S:555:HOH:O	2.02	0.59	
13:S:501:HOH:O	2:L:178:GLN:HB2	2.03	0.59	
2:M:500[B]:ARG:NH2	13:M:707:HOH:O	2.36	0.57	
2:L:179:LEU:HD13	13:L:804:HOH:O	2.04	0.57	
2:M:472:LYS:HE3	13:M:715:HOH:O	2.07	0.55	
2:L:457:HIS:HB3	13:L:825:HOH:O	2.07	0.55	
2:M:530:VAL:CG1	2:M:531:PRO:HD2	2.38	0.53	
2:M:509:ARG:CZ	11:M:604:CMO:O	2.57	0.53	
2:L:333[B]:ASN:ND2	2:L:335:LEU:HD21	2.23	0.53	
2:L:275[B]:MET:HE3	2:L:456:ALA:HA	1.93	0.51	
1:T:186:ILE:HD11	1:T:228:ASN:HB3	1.93	0.51	
2:L:179:LEU:CD1	13:L:804:HOH:O	2.58	0.51	
2:L:144:LYS:HB3	2:L:197[A]:GLU:HG2	1.94	0.50	
2:M:243:ILE:HG23	2:M:254:MET:HG2	1.94	0.49	
1:T:66:GLN:OE1	13:T:502:HOH:O	2.20	0.48	
2:L:530:VAL:CG1	2:L:531:PRO:HD2	2.43	0.48	
2:L:576:CYS:HB2	11:L:605:CMO:C	2.43	0.48	
2:L:4:GLN:HA	2:L:12:ILE:O	2.14	0.47	
1:S:186:ILE:HD11	1:S:228:ASN:HB3	1.97	0.47	
2:L:540:ASP:HB2	2:L:541:PRO:CD	2.44	0.47	
2:M:300:CYS:HA	2:M:326:VAL:O	2.15	0.47	
1:T:266:ARG:NE	1:T:266:ARG:HA	2.30	0.47	
2:M:540:ASP:HB2	2:M:541:PRO:CD	2.44	0.46	
2:M:535:ASN:HB3	2:M:548:TYR:CE1	2.52	0.45	
2:L:576:CYS:CB	11:L:605:CMO:C	2.92	0.45	
2:L:391:GLU:HA	2:L:395:TYR:CD2	2.51	0.45	
1:T:93:ARG:NH2	1:T:97:GLU:OE1	2.49	0.45	
2:L:256[B]:ARG:HD3	13:L:1083:HOH:O	2.16	0.45	
2:L:243:ILE:HG23	2:L:254:MET:HG2	1.98	0.44	
1:S:177:ARG:NH1	13:S:507:HOH:O	2.45	0.44	
1:S:111:ALA:HB2	1:S:134[B]:ILE:HD11	2.00	0.44	
1:S:244:GLN:HE21	2:L:256[B]:ARG:NH1	2.17	0.43	
2:L:445:ILE:O	2:L:450:GLY:HA3	2.18	0.43	
2:L:275[B]:MET:HE2	2:L:456:ALA:HA	1.99	0.43	

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Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:M:63:ARG:HB2	2:M:523[B]:ILE:HD12	2.00	0.43
2:L:535:ASN:HB3	2:L:548:TYR:CE1	2.54	0.42
2:M:509:ARG:NH1	11:M:604:CMO:O	2.53	0.42
2:M:536:ALA:HB2	2:M:548:TYR:CE2	2.55	0.42
2:M:576:CYS:CB	11:M:604:CMO:C	2.97	0.42
2:L:14:ASN:ND2	13:L:711:HOH:O	2.51	0.42
2:M:60:LEU:HD12	2:M:523[B]:ILE:HD13	2.01	0.42
2:M:530:VAL:HG12	2:M:531:PRO:HD2	2.02	0.41
1:T:260:ARG:HG3	13:T:514:HOH:O	2.20	0.41
1:S:241:PHE:CE2	1:S:243:ILE:HB	2.56	0.41
1:S:7:ILE:HA	1:S:8:PRO:HD3	1.95	0.41
2:M:492:PRO:HA	2:M:495:TRP:CD2	2.56	0.40
2:L:3:THR:HG23	13:L:1024:HOH:O	2.21	0.40
2:M:172:LYS:O	2:M:175[A]:GLU:HG2	2.22	0.40
2:M:272:ASN:OD1	2:M:460:GLN:HG3	2.21	0.40
1:S:223:GLY:N	1:S:224:PRO:CD	2.85	0.40

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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	S	265/279~(95%)	253~(96%)	12 (4%)	0	100	100
1	Т	269/279~(96%)	259~(96%)	10 (4%)	0	100	100
2	L	593/582~(102%)	577~(97%)	16 (3%)	0	100	100
2	М	592/582~(102%)	576~(97%)	16 (3%)	0	100	100
All	All	1719/1722~(100%)	1665 (97%)	54 (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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Rotameric Outliers		Percentiles		
1	S	220/232~(95%)	219 (100%)	1 (0%)	86	71		
1	Т	224/232~(97%)	223 (100%)	1 (0%)	89	76		
2	L	492/481~(102%)	491 (100%)	1 (0%)	92	79		
2	М	493/481~(102%)	493 (100%)	0	100	100		
All	All	1429/1426 (100%)	1426 (100%)	3 (0%)	92	79		

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

Mol	Chain	\mathbf{Res}	Type
1	S	191	TYR
2	L	6	GLU
1	Т	126	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	203	GLN
2	L	328	ASN
2	L	388	GLN
2	М	479	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 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	Type	Chain	Dog	Link	B	ond leng	gths	B	ond ang	gles
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	F3S	S	402	1	0,9,9	-	-	-		
3	SF4	S	401	1	0,12,12	-	-	-		
5	SF3	Т	403	1	0,8,8	-	-	-		
11	CMO	L	605	-	0,1,1	-	-	-		
5	SF3	S	403	1	0,8,8	-	-	-		
8	FCO	L	602	2	0,6,6	-	-	-		
12	TRS	L	606	-	7,7,7	0.32	0	$9,\!9,\!9$	0.36	0
4	F3S	Т	402	1	0,9,9	-	-	-		•
11	CMO	М	604	9	0,1,1	-	-	-		
8	FCO	М	601	2	0,6,6	-	-	-		
3	SF4	Т	401	1	0,12,12	-	-	-		
7	SO4	L	601	-	4,4,4	0.48	0	$6,\!6,\!6$	0.30	0
7	SO4	М	605	-	4,4,4	0.17	0	$6,\!6,\!6$	0.21	0
7	SO4	Т	406	-	4,4,4	0.16	0	6,6,6	0.22	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
4	F3S	S	402	1	-	-	0/3/3/3
3	SF4	S	401	1	-	-	0/6/5/5
5	SF3	Т	403	1	-	-	0/2/2/2
5	SF3	S	403	1	-	-	0/2/2/2
12	TRS	L	606	-	-	3/9/9/9	-
4	F3S	Т	402	1	-	-	0/3/3/3



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	Т	401	1	-	-	0/6/5/5

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
12	L	606	TRS	C1-C-C2-O2
12	L	606	TRS	C3-C-C2-O2
12	L	606	TRS	N-C-C2-O2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	605	CMO	5	0
11	М	604	CMO	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	S	263/279~(94%)	-0.11	5 (1%) 66 67	9, 17, 29, 79	4 (1%)
1	Т	263/279~(94%)	-0.02	4 (1%) 71 74	9, 17, 30, 74	8 (3%)
2	L	581/582~(99%)	-0.03	11 (1%) 66 67	8, 18, 33, 68	13 (2%)
2	М	581/582~(99%)	-0.08	4 (0%) 84 86	7, 18, 28, 47	13 (2%)
All	All	1688/1722~(98%)	-0.06	24 (1%) 73 75	7, 18, 31, 79	38 (2%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	177[A]	GLY	3.7
1	Т	4	LYS	3.3
1	S	4	LYS	3.3
1	S	5	PRO	3.1
2	L	425	ALA	3.0
1	Т	66	GLN	3.0
2	L	428	VAL	2.9
1	Т	62	ASP	2.8
1	S	7	ILE	2.8
2	М	3	THR	2.7
2	L	442	LEU	2.5
2	L	437	ALA	2.4
2	М	2	SER	2.3
2	L	433	ARG	2.3
2	L	431	VAL	2.3
2	L	430	SER	2.3
2	L	440	LEU	2.2
1	S	260	ARG	2.2
1	S	6	ARG	2.1
2	М	373	TRP	2.1
2	М	332	ASN	2.1



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Mol	Chain	\mathbf{Res}	Type	RSRZ
1	Т	5	PRO	2.1
2	L	3	THR	2.0
2	L	176	GLY	2.0

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 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
11	CMO	L	605	2/2	0.66	0.22	$44,\!44,\!44,\!57$	0
11	CMO	М	604	2/2	0.66	0.41	37,37,37,45	0
12	TRS	L	606	8/8	0.87	0.11	28,32,35,36	0
7	SO4	М	605	5/5	0.88	0.12	23,32,36,36	0
7	SO4	Т	406	5/5	0.92	0.10	22,32,37,42	0
7	SO4	L	601	5/5	0.97	0.07	22,23,27,27	5
6	CL	Т	404	1/1	0.99	0.06	21,21,21,21	0
9	NI	L	603	1/1	0.99	0.06	20,20,20,20	0
9	NI	М	602	1/1	0.99	0.04	20,20,20,20	0
6	CL	Т	405	1/1	0.99	0.04	20,20,20,20	0
6	CL	S	404	1/1	0.99	0.07	21,21,21,21	0
6	CL	S	405	1/1	0.99	0.04	21,21,21,21	0
3	SF4	S	401	8/8	1.00	0.02	$14,\!15,\!15,\!15$	0
8	FCO	L	602	7/7	1.00	0.03	$14,\!14,\!15,\!16$	0
8	FCO	М	601	7/7	1.00	0.04	14,15,16,16	0
3	SF4	Т	401	8/8	1.00	0.02	$14,\!14,\!15,\!15$	0
4	F3S	S	402	7/7	1.00	0.01	13,13,14,14	0
10	MG	L	604	1/1	1.00	0.01	14,14,14,14	0
10	MG	М	603	1/1	1.00	0.03	13,13,13,13	0
4	F3S	Т	402	7/7	1.00	0.02	13,14,14,14	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
5	SF3	S	403	7/7	1.00	0.01	14, 14, 14, 14	0
5	SF3	Т	403	7/7	1.00	0.02	14,14,15,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.















6.5 Other polymers (i)

There are no such residues in this entry.

