

Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2022 – 06:40 pm GMT

PDB ID : 7NEM

Title: Hydrogenase-2 variant R479K - anaerobically oxidised form

Authors : Carr, S.B. Deposited on : 2021-02-04

Resolution : 1.35 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 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 : 2.26

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

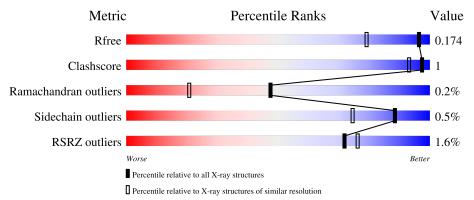
Validation Pipeline (wwPDB-VP) : 2.26

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 1.35 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 $(\# \mathrm{Entries})$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	298	88%	• 10%
1	Т	298	89%	• 10%
2	L	567	95%	
2	M	567	93%	



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14108 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-2 small chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	S	268	Total 2050	C 1299	N 360	O 378	S 13	0	2	0
1	Т	268	Total 2050	C 1299	N 360	O 378	S 13	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	294	HIS	-	expression tag	UNP P69741
S	295	HIS	-	expression tag	UNP P69741
S	296	HIS	-	expression tag	UNP P69741
S	297	HIS	-	expression tag	UNP P69741
S	298	HIS	-	expression tag	UNP P69741
S	299	HIS	-	expression tag	UNP P69741
Т	294	HIS	_	expression tag	UNP P69741
Т	295	HIS	-	expression tag	UNP P69741
Т	296	HIS	_	expression tag	UNP P69741
Т	297	HIS	-	expression tag	UNP P69741
Т	298	HIS	-	expression tag	UNP P69741
Т	299	HIS	_	expression tag	UNP P69741

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

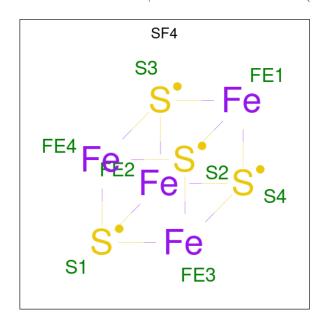
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	Т	551	Total	С	N	О	S	0	9	0
	ь	991	4298	2736	736	808	18	0	3	
9	M	551	Total	С	N	О	S	0	G	0
	IVI	991	4318	2749	741	810	18	U	0	

There are 2 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
L	479	LYS	ARG	engineered mutation	UNP P0ACE0
M	479	LYS	ARG	engineered mutation	UNP P0ACE0

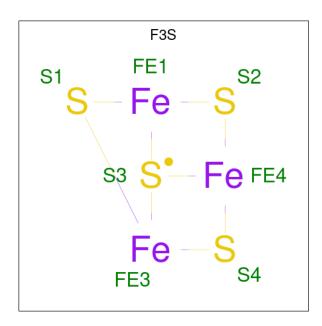
 \bullet Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atom	\mathbf{s}	ZeroOcc	AltConf	
3	S	1	Total Fe	e S	0	0	
3	Σ	1	8 4	4	O		
3	Q	1	Total Fe	e S	0	0	
J	D	1	8 4	4	U	U	
3	Т	1	Total Fe	e S	0	0	
3	1	1	8 4	4	0	U	
2	Т	1	Total Fe	e S	0	0	
3	1	1	8 4	4		0	

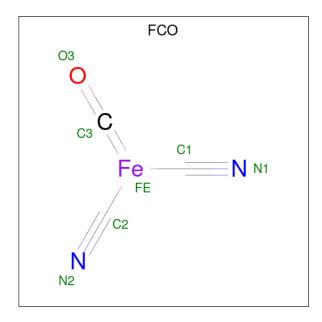
• Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	1	Total Fe S 7 3 4	0	0
4	Т	1	Total Fe S 7 3 4	0	0

• Molecule 5 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues		$\mathbf{A}\mathbf{t}$	oms			ZeroOcc	AltConf
5	L	1	Total 7	C 3	Fe 1	N 2	O 1	0	0



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	М	1	Total 7	C 3	Fe 1	N 2	O 1	0	0

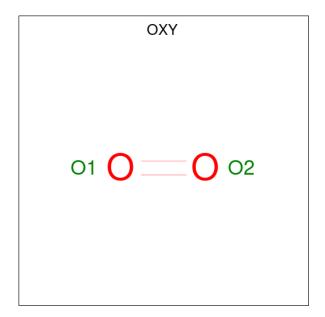
• Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total Ni 1 1	0	0
6	M	1	Total Ni 1 1	0	0

• Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	2	Total Mg 2 2	0	0
7	M	2	Total Mg 2 2	0	0

• Molecule 8 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total O 2 2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total O 2 2	0	0

• Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Cl 1 1	0	0

• Molecule 10 is water.

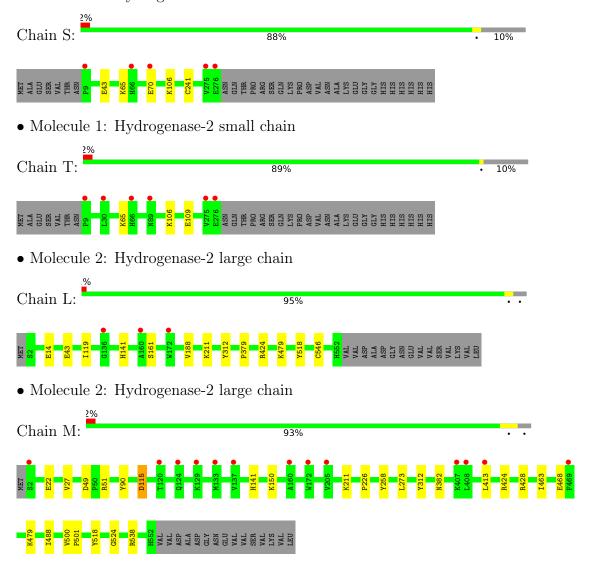
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	S	230	Total O 230 230	0	0
10	L	475	Total O 475 475	0	0
10	Т	199	Total O 199 199	0	0
10	M	417	Total O 417 417	0	0



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-2 small chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	99.40Å 100.25Å 168.54Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.80 - 1.35	Depositor
Resolution (A)	44.76 - 1.35	EDS
% Data completeness	99.9 (44.80-1.35)	Depositor
(in resolution range)	$100.0 \ (44.76 - 1.35)$	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.45 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.150 , 0.167	Depositor
it, it _{free}	0.160 , 0.174	DCC
R_{free} test set	18274 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14108	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.58% 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: FCO, OXY, CL, SF4, F3S, NI, MG

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	Mol Chain		nd lengths	Bond angles	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	S	0.80	2/2114 (0.1%)	0.88	0/2878
1	Т	0.76	0/2114	0.89	0/2878
2	L	0.73	1/4414 (0.0%)	0.89	3/6016 (0.0%)
2	M	0.73	0/4440	0.89	8/6051 (0.1%)
All	All	0.74	3/13082 (0.0%)	0.89	11/17823 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
2	L	43	GLU	CD-OE1	6.27	1.32	1.25
1	S	43[A]	GLU	C-O	5.30	1.33	1.23
1	S	43[B]	GLU	C-O	5.30	1.33	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	M	424	ARG	NE-CZ-NH2	-8.50	116.05	120.30
2	L	424	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	M	428	ARG	NE-CZ-NH2	-6.62	116.99	120.30
2	L	518	TYR	CB-CG-CD2	-6.41	117.15	121.00
2	M	424	ARG	NE-CZ-NH1	6.35	123.48	120.30
2	M	518	TYR	CB-CG-CD2	-6.04	117.37	121.00
2	L	518	TYR	CB-CG-CD1	5.99	124.59	121.00
2	M	382	ASN	N-CA-CB	-5.32	101.02	110.60
2	M	90	TYR	CB-CG-CD2	-5.29	117.82	121.00
2	M	115	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	M	258	TYR	CB-CG-CD1	5.05	124.03	121.00

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	S	2050	0	1974	4	0
1	Т	2050	0	1974	2	0
2	L	4298	0	4241	4	0
2	M	4318	0	4268	10	0
3	S	16	0	0	0	0
3	Τ	16	0	0	0	0
4	S	7	0	0	0	0
4	Τ	7	0	0	0	0
5	L	7	0	0	0	0
5	M	7	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
7	L	2	0	0	0	0
7	M	2	0	0	0	0
8	L	2	0	0	0	0
8	M	2	0	0	0	0
9	M	1	0	0	0	0
10	L	475	0	0	3	4
10	M	417	0	0	2	2
10	S	230	0	0	3	0
10	Τ	199	0	0	2	1
All	All	14108	0	12457	20	4

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 1.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
2:M:150:LYS:HE3	10:M:888:HOH:O	1.47	1.10
1:S:70:GLU:HG2	10:S:622:HOH:O	1.84	0.77
1:S:241:CYS:SG	10:L:1062:HOH:O	2.44	0.76
2:M:22:GLU:HG3	10:M:1070:HOH:O	1.87	0.73
1:T:109:GLU:HG2	10:T:686:HOH:O	1.89	0.71
2:M:500:VAL:CG1	2:M:501:PRO:HD2	2.42	0.49



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:S:106:LYS:HE3	10:S:710:HOH:O	2.15	0.46
2:M:49:ASP:OD2	2:M:51[B]:ARG:NH2	2.44	0.46
1:S:65:LYS:HE3	10:S:502:HOH:O	2.17	0.45
2:M:273:LEU:HD22	2:M:413:LEU:HD21	1.98	0.44
2:M:51[B]:ARG:CZ	2:M:463:ILE:HD12	2.48	0.43
1:T:106:LYS:HD3	10:T:666:HOH:O	2.19	0.43
2:L:379:PRO:HA	10:L:1072:HOH:O	2.20	0.41
2:M:27:VAL:CG1	2:M:524:GLY:HA2	2.51	0.41
2:L:119:ILE:CD1	2:L:188:VAL:HG22	2.51	0.41
2:M:115:ASP:HB3	2:M:538:ARG:HG2	2.03	0.41
2:L:14:GLU:HB3	2:L:546:CYS:HA	2.04	0.40
2:L:161:SER:HB2	10:L:839:HOH:O	2.21	0.40
2:M:500:VAL:HG13	2:M:501:PRO:HD2	2.02	0.40
2:M:468:GLU:HA	2:M:488:ILE:O	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
10:L:786:HOH:O	10:M:1052:HOH:O[4_465]	1.09	1.11
10:L:714:HOH:O	10:L:857:HOH:O[3_755]	1.12	1.08
10:L:1031:HOH:O	10:M:1052:HOH:O[4_465]	2.13	0.07
10:L:767:HOH:O	10:T:510:HOH:O[4_475]	2.16	0.04

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	268/298 (90%)	257 (96%)	11 (4%)	0	100	100
1	Т	268/298 (90%)	258 (96%)	10 (4%)	0	100	100
2	L	552/567 (97%)	529 (96%)	22 (4%)	1 (0%)	47	21



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percenti	les
2	M	555/567 (98%)	533 (96%)	20 (4%)	2 (0%)	34 12	2
All	All	1643/1730 (95%)	1577 (96%)	63 (4%)	3 (0%)	47 21	

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	211	LYS
2	L	211	LYS
2	M	226	PRO

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	S	215/239~(90%)	215 (100%)	0	100	100
1	Т	215/239 (90%)	214 (100%)	1 (0%)	88	74
2	L	468/479 (98%)	465 (99%)	3 (1%)	86	69
2	M	471/479 (98%)	468 (99%)	3 (1%)	86	69
All	All	1369/1436 (95%)	1362 (100%)	7 (0%)	88	74

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	141	HIS
2	L	312	TYR
2	L	479	LYS
1	Т	65	LYS
2	M	141	HIS
2	M	312	TYR
2	M	479	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
2	L	47	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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).

Mol	Type	Chain	Res	Link	В	ond leng	$_{ m gths}$	В	ond angles
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	$\mid \text{RMSZ} \mid \# Z > 2$
3	SF4	Т	403	1	0,12,12	-	-	-	
5	FCO	M	601	2	0,6,6	-	-	-	
4	F3S	S	402	1	0,9,9	-	-	-	
8	OXY	M	606	-	1,1,1	0.02	0	-	
8	OXY	L	605	6	1,1,1	0.12	0	-	
5	FCO	L	601	2	0,6,6	-	-	-	
3	SF4	Т	401	1	0,12,12	-	-	-	
4	F3S	Т	402	1	0,9,9	-	-	-	
3	SF4	S	401	1	0,12,12	-	-	-	
3	SF4	S	403	1	0,12,12	-	-	-	

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.



, ,		. 1.	C 11 1	1 • 1		1 1.0 1
'-' means	no	outhers	of that	, kind	were	identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	Т	403	1	-	-	0/6/5/5
4	F3S	S	402	1	-	-	0/3/3/3
3	SF4	Т	401	1	-	-	0/6/5/5
4	F3S	Т	402	1	-	-	0/3/3/3
3	SF4	S	401	1	-	-	0/6/5/5
3	SF4	S	403	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

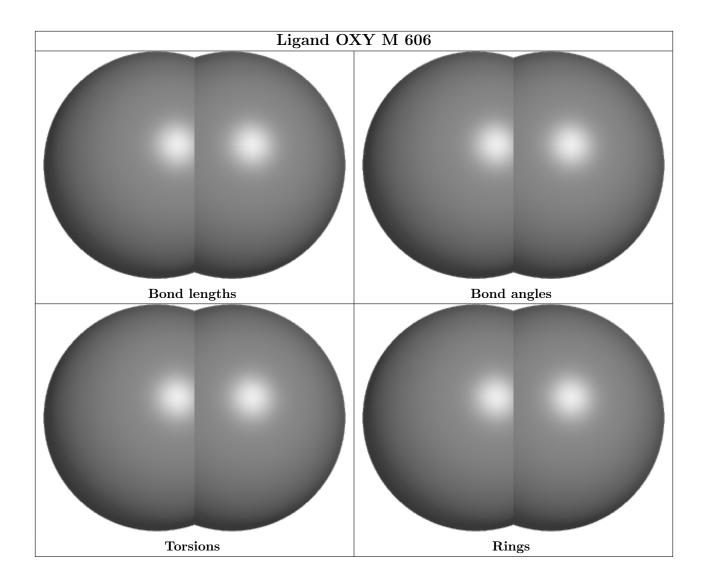
There are no torsion outliers.

There are no ring outliers.

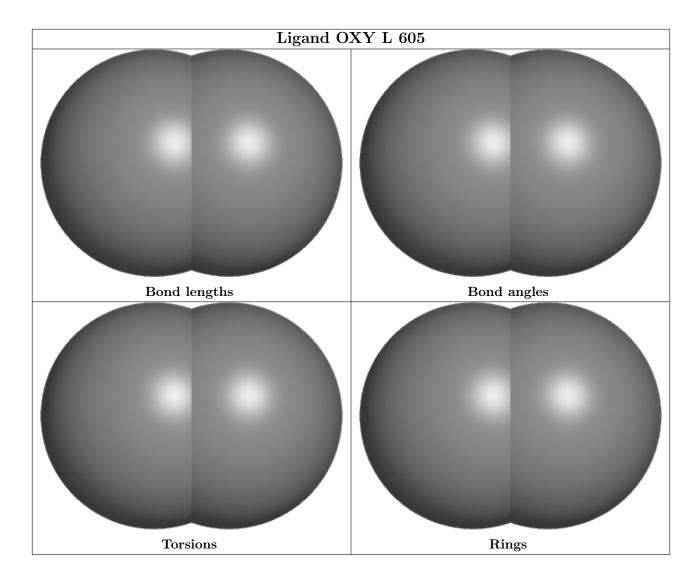
No monomer is involved in short contacts.

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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	S	$268/298 \ (89\%)$	-0.08	5 (1%) 66 71	9, 13, 26, 45	0
1	Т	268/298 (89%)	0.08	6 (2%) 62 68	10, 15, 28, 47	0
2	L	551/567 (97%)	-0.17	3 (0%) 91 92	9, 13, 25, 36	0
2	M	551/567 (97%)	0.03	13 (2%) 59 65	9, 14, 28, 43	0
All	All	1638/1730 (94%)	-0.05	27 (1%) 72 76	9, 13, 27, 47	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	172	TRP	5.5
1	Т	9	PRO	5.2
1	S	9	PRO	5.1
1	Т	275	VAL	4.9
2	L	172	TRP	3.8
1	S	275	VAL	3.8
1	S	276	GLU	3.7
1	Т	276	GLU	3.6
2	M	160	ALA	2.8
2	M	205	VAL	2.6
1	Т	89	ASN	2.6
2	M	129	LYS	2.6
2	L	136	GLY	2.5
2	L	160	ALA	2.5
2	M	408	LEU	2.4
1	S	66	HIS	2.4
1	Т	30	LEU	2.4
2	M	407	LYS	2.4
1	S	70	GLU	2.3
1	Т	66	HIS	2.3
2	M	469	PHE	2.2



Mol	Chain	Res	Type	RSRZ
2	M	413	LEU	2.2
2	M	133	MET	2.2
2	M	124	GLN	2.1
2	M	137	VAL	2.1
2	M	120	THR	2.0
2	M	2	SER	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.

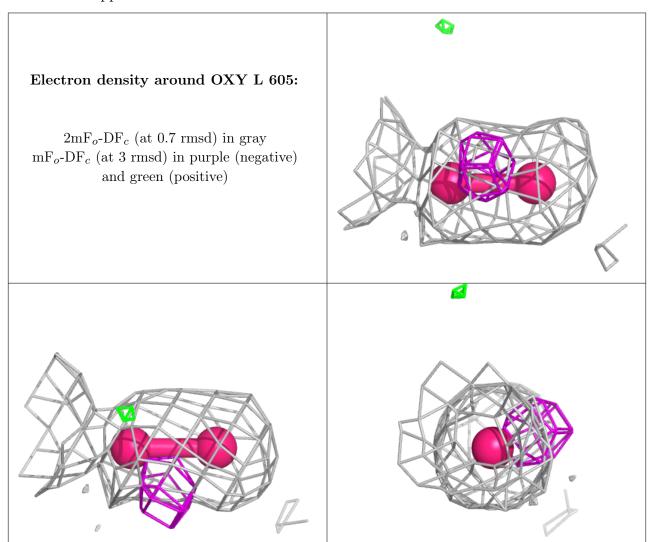
6.4 Ligands (i)

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.

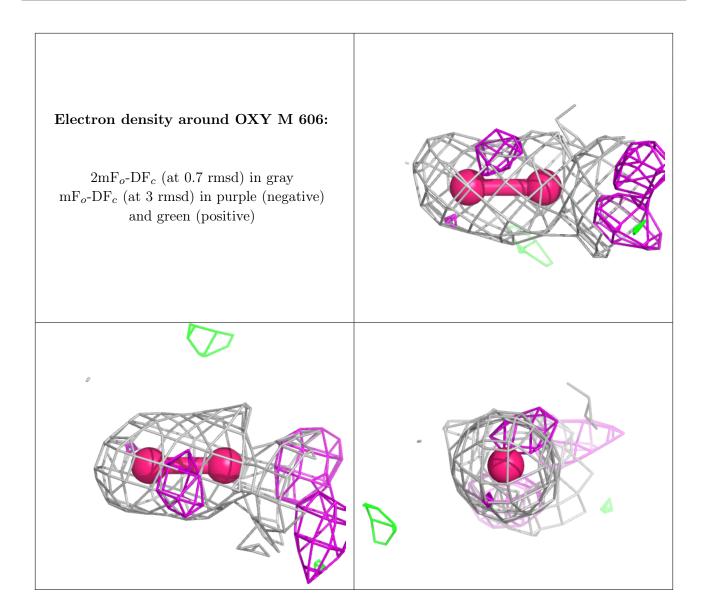
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q<0.9
7	MG	L	604	1/1	0.97	0.20	29,29,29,29	0
8	OXY	L	605	2/2	0.97	0.12	16,16,16,18	0
8	OXY	M	606	2/2	0.97	0.12	20,20,20,23	0
7	MG	Μ	604	1/1	0.99	0.24	23,23,23,23	0
9	CL	M	605	1/1	0.99	0.04	19,19,19,19	0
4	F3S	Τ	402	7/7	1.00	0.05	10,10,10,10	0
5	FCO	L	601	7/7	1.00	0.06	8,9,10,11	0
5	FCO	M	601	7/7	1.00	0.07	9,10,11,11	0
6	NI	L	602	1/1	1.00	0.04	10,10,10,10	0
6	NI	M	602	1/1	1.00	0.04	11,11,11,11	0
7	MG	L	603	1/1	1.00	0.09	6,6,6,6	0
3	SF4	S	401	8/8	1.00	0.04	10,11,11,11	0
7	MG	M	603	1/1	1.00	0.08	8,8,8,8	0
3	SF4	S	403	8/8	1.00	0.05	9,9,10,10	0
3	SF4	Т	401	8/8	1.00	0.04	11,11,11,11	0
3	SF4	Т	403	8/8	1.00	0.05	10,11,11,11	0
4	F3S	S	402	7/7	1.00	0.05	9,9,10,10	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.

