Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2022 – 09:12 pm GMT

PDB ID	:	7PES
Title	:	Crystal Structure of Two-Domain Laccase mutant M199G from Streptomyces griseoflavus
Authors	:	Gabdulkhakov, A.; Tishchenko, S.; Kolyadenko, I.
Deposited on	:	2021-08-11
Resolution	:	1.75 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 ⓘ symbol.

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

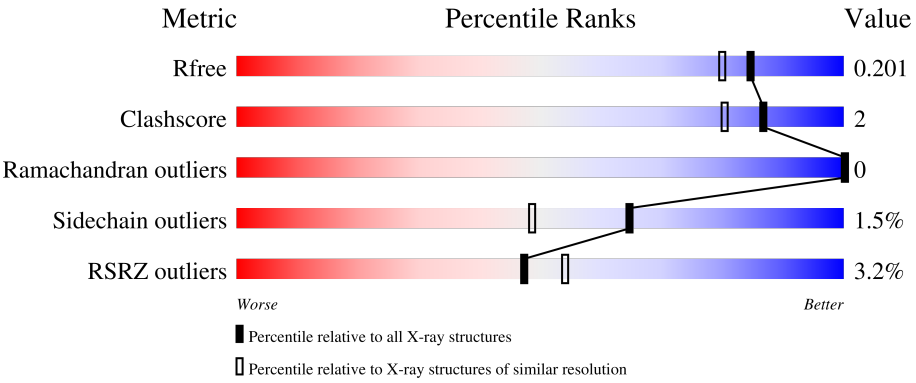
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 1.75 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	283	4% 93% 5% ·
1	B	283	4% 88% 10% ·
1	C	283	2% 91% 7% ·
1	D	283	4% 94% · ·
1	E	283	3% 91% 7% ·

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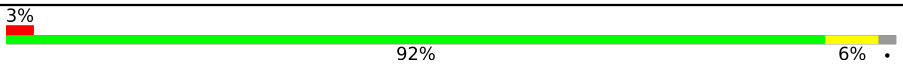
Mol	Chain	Length	Quality of chain
1	F	283	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13900 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 Two-domain laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total 2150	C 1341	N 393	O 405	S 11	0	3	0
1	B	277	Total 2173	C 1354	N 400	O 407	S 12	0	6	0
1	C	277	Total 2191	C 1362	N 404	O 412	S 13	0	8	0
1	D	279	Total 2182	C 1359	N 402	O 409	S 12	0	6	0
1	E	277	Total 2160	C 1346	N 396	O 406	S 12	0	5	0
1	F	277	Total 2164	C 1348	N 396	O 408	S 12	1	5	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
B	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
C	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
D	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
E	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
F	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Cu 4	0	0
2	B	5	Total 5	Cu 5	1	0
2	C	3	Total 3	Cu 3	0	0

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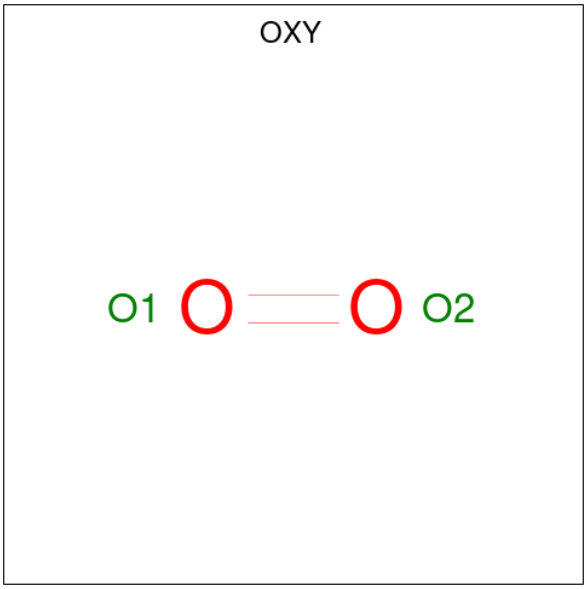
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	4	Total Cu 4 4	0	0
2	E	3	Total Cu 3 3	0	0
2	F	5	Total Cu 5 5	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O 2 2	0	0
4	E	1	Total O 2 2	0	0

- Molecule 5 is water.

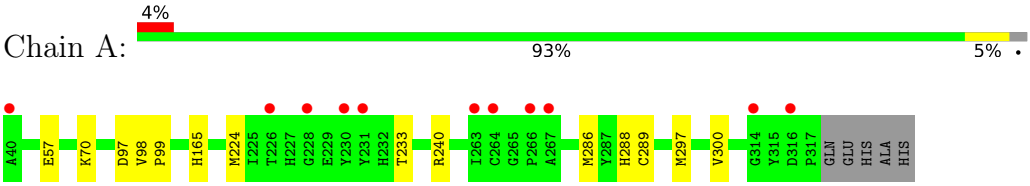
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	167	Total O 167 167	0	0
5	B	129	Total O 129 129	0	0
5	C	135	Total O 135 135	0	0
5	D	134	Total O 134 134	0	0
5	E	125	Total O 125 125	0	0
5	F	158	Total O 158 158	0	0

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.

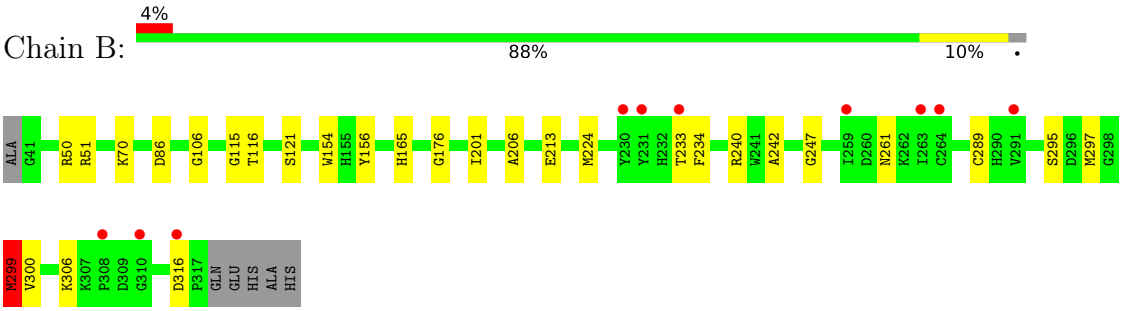
• Molecule 1: Two-domain laccase

Chain A:



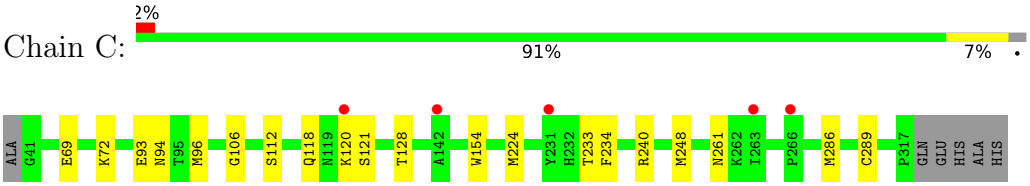
• Molecule 1: Two-domain laccase

Chain B:



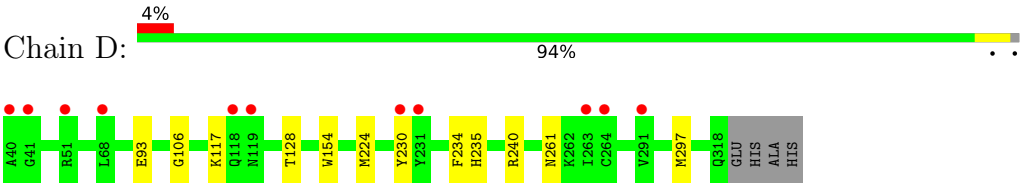
• Molecule 1: Two-domain laccase

Chain C:



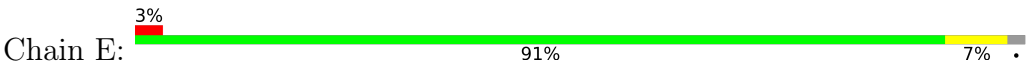
• Molecule 1: Two-domain laccase

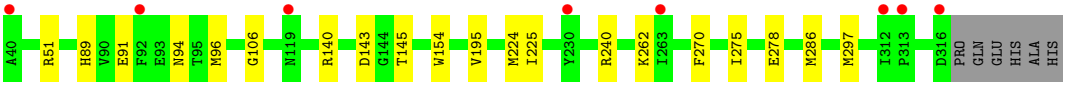
Chain D:



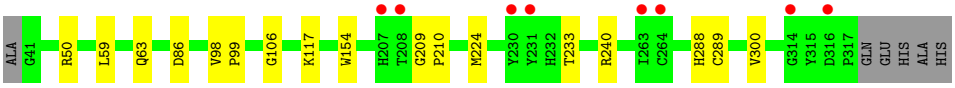
• Molecule 1: Two-domain laccase

Chain E:





• Molecule 1: Two-domain laccase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.17Å 94.36Å 119.80Å 90.00° 91.14° 90.00°	Depositor
Resolution (Å)	47.18 – 1.75 47.18 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.18-1.75) 99.0 (47.18-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.8.0230, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.166 , 0.201 0.170 , 0.201	Depositor DCC
R_{free} test set	1970 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	13900	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: OXY, CU, NA

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	0.39	0/2212	0.64	0/3006
1	B	0.38	0/2235	0.66	1/3036 (0.0%)
1	C	0.38	0/2253	0.63	0/3056
1	D	0.39	0/2244	0.65	0/3047
1	E	0.36	0/2221	0.63	0/3016
1	F	0.40	0/2226	0.64	0/3023
All	All	0.38	0/13391	0.64	1/18184 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	299	MET	CA-CB-CG	5.02	121.84	113.30

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	2150	0	2020	9	0
1	B	2173	0	2047	14	0
1	C	2191	0	2058	11	0
1	D	2182	0	2051	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2160	0	2032	11	0
1	F	2164	0	2031	9	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
2	E	3	0	0	0	0
2	F	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
5	A	167	0	0	1	0
5	B	129	0	0	1	0
5	C	135	0	0	3	0
5	D	134	0	0	1	0
5	E	125	0	0	1	0
5	F	158	0	0	0	0
All	All	13900	0	12239	54	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 (54) 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:213:GLU:OE1	1:B:306:LYS:NZ	2.36	0.58
1:B:50:ARG:NH2	1:B:86:ASP:OD2	2.37	0.58
1:B:165:HIS:HD2	5:C:505:HOH:O	1.88	0.56
1:A:288:HIS:HB3	1:A:300[A]:VAL:HG13	1.86	0.56
1:C:94:ASN:OD1	1:C:96:MET:HB2	2.06	0.56
1:D:93:GLU:HG3	1:D:128:THR:HG22	1.89	0.54
1:B:115:GLY:H	1:B:121:SER:HB3	1.71	0.54
5:B:501:HOH:O	1:C:286:MET:HG3	2.06	0.54
5:D:502:HOH:O	1:E:286:MET:HG3	2.08	0.54
1:C:112:SER:O	1:C:121[B]:SER:OG	2.27	0.53
1:E:94:ASN:OD1	1:E:96:MET:HB2	2.09	0.53
1:E:143:ASP:OD1	1:E:145:THR:OG1	2.22	0.51
1:C:69[B]:GLU:HB2	1:C:72:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLY:HA3	1:D:154:TRP:CD2	2.46	0.50
1:C:248[B]:MET:HG2	5:C:561:HOH:O	2.12	0.49
1:B:242:ALA:O	1:B:247:GLY:HA2	2.13	0.48
1:D:235:HIS:HB2	1:D:261:ASN:OD1	2.14	0.47
1:E:51:ARG:NH2	1:E:91:GLU:OE1	2.36	0.47
1:A:233:THR:O	1:A:289:CYS:HA	2.15	0.46
1:B:206:ALA:HB1	1:B:297:MET:O	2.16	0.46
1:C:234:PHE:O	1:C:261:ASN:HA	2.16	0.46
1:A:99:PRO:HD2	1:F:98:VAL:HG12	1.97	0.45
1:A:286:MET:HG3	5:C:535:HOH:O	2.16	0.45
1:C:93:GLU:HG3	1:C:128:THR:HG22	1.98	0.44
1:A:57:GLU:OE1	5:A:501:HOH:O	2.21	0.44
1:B:233:THR:O	1:B:289:CYS:HA	2.16	0.44
1:E:262:LYS:HD3	1:E:270:PHE:CZ	2.53	0.44
1:A:297:MET:HG3	1:D:230:TYR:OH	2.18	0.43
1:F:59:LEU:HB2	1:F:63:GLN:HB2	2.00	0.43
1:F:233:THR:O	1:F:289:CYS:HA	2.19	0.43
1:F:106:GLY:HA3	1:F:154:TRP:CD2	2.54	0.42
1:F:209:GLY:HA3	1:F:210:PRO:HA	1.93	0.42
1:A:165:HIS:CE1	1:B:300[B]:VAL:HG11	2.54	0.42
1:B:106:GLY:HA3	1:B:154:TRP:CD2	2.53	0.42
1:E:106:GLY:HA3	1:E:154:TRP:CD2	2.54	0.42
1:B:116:THR:H	1:B:121:SER:HB2	1.84	0.42
1:E:297:MET:HE1	5:E:551:HOH:O	2.18	0.42
1:C:106:GLY:HA3	1:C:154:TRP:CD2	2.55	0.42
1:B:201:ILE:HG13	1:B:299:MET:HB3	2.02	0.42
1:F:288:HIS:HB3	1:F:300:VAL:HG12	2.00	0.42
1:E:140:ARG:HD3	1:E:140:ARG:HA	1.80	0.42
1:A:97:ASP:OD2	1:F:117:LYS:HE3	2.19	0.41
1:B:234:PHE:O	1:B:261:ASN:HA	2.20	0.41
1:C:69[A]:GLU:HB3	1:C:72:LYS:HE2	2.01	0.41
1:F:50:ARG:NH2	1:F:86:ASP:OD2	2.53	0.41
1:C:118:GLN:OE1	1:C:118:GLN:N	2.46	0.41
1:A:98:VAL:HG12	1:F:99:PRO:HD2	2.02	0.41
1:E:195:VAL:HA	1:E:225:ILE:O	2.21	0.41
1:B:289:CYS:O	1:B:295:SER:HB3	2.21	0.40
1:D:234:PHE:O	1:D:261:ASN:HA	2.21	0.40
1:E:275:ILE:HB	1:E:278:GLU:HB2	2.03	0.40
1:C:233:THR:O	1:C:289:CYS:HA	2.21	0.40
1:E:51:ARG:HG2	1:E:89:HIS:HB2	2.03	0.40
1:B:156:TYR:CZ	1:B:176:GLY:HA3	2.57	0.40

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	Percentiles	
1	A	279/283 (99%)	276 (99%)	3 (1%)	0	100	100
1	B	281/283 (99%)	274 (98%)	7 (2%)	0	100	100
1	C	283/283 (100%)	278 (98%)	5 (2%)	0	100	100
1	D	283/283 (100%)	278 (98%)	5 (2%)	0	100	100
1	E	280/283 (99%)	272 (97%)	8 (3%)	0	100	100
1	F	280/283 (99%)	275 (98%)	5 (2%)	0	100	100
All	All	1686/1698 (99%)	1653 (98%)	33 (2%)	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	Percentiles	
1	A	221/222 (100%)	218 (99%)	3 (1%)	67	52
1	B	224/222 (101%)	218 (97%)	6 (3%)	44	22
1	C	226/222 (102%)	222 (98%)	4 (2%)	59	40
1	D	224/222 (101%)	220 (98%)	4 (2%)	59	40
1	E	222/222 (100%)	220 (99%)	2 (1%)	78	67
1	F	223/222 (100%)	220 (99%)	3 (1%)	69	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1340/1332 (101%)	1318 (98%)	22 (2%)	65 45

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	224	MET
1	A	240	ARG
1	B	51	ARG
1	B	70	LYS
1	B	224	MET
1	B	240	ARG
1	B	299	MET
1	B	316	ASP
1	C	120[A]	LYS
1	C	120[B]	LYS
1	C	224	MET
1	C	240	ARG
1	D	117	LYS
1	D	224	MET
1	D	240	ARG
1	D	297	MET
1	E	224	MET
1	E	240	ARG
1	F	224[A]	MET
1	F	224[B]	MET
1	F	240	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 28 are monoatomic - leaving 2 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	OXY	E	404	2	1,1,1	0.16	0	-		
4	OXY	C	404	2	1,1,1	0.10	0	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

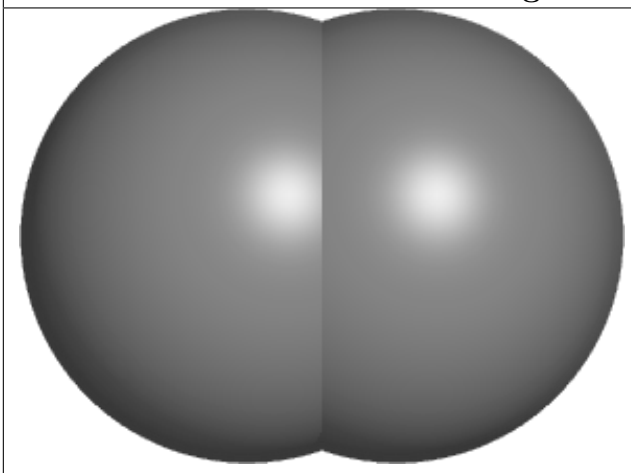
There are no torsion outliers.

There are no ring outliers.

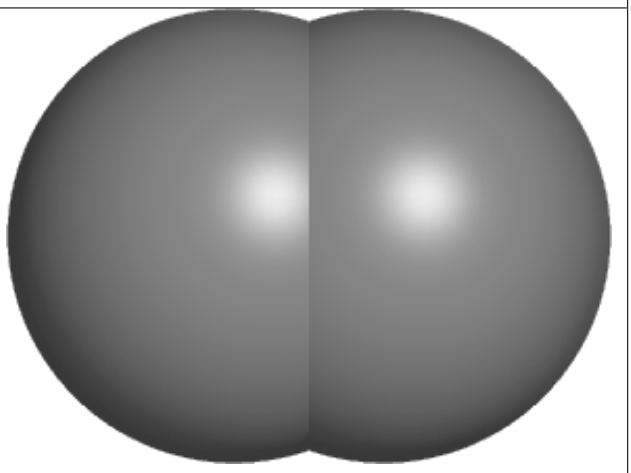
No monomer is involved in short contacts.

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.

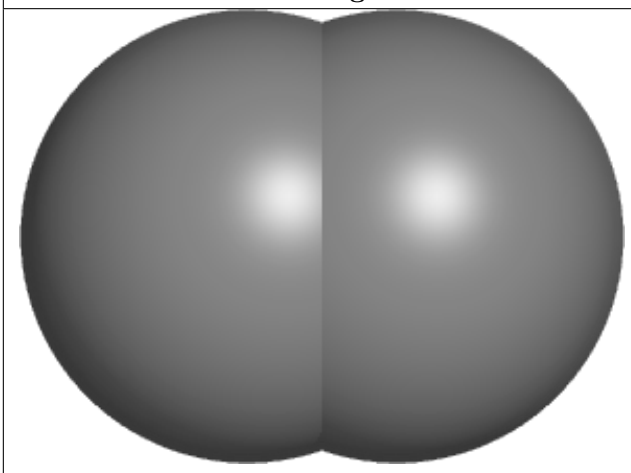
Ligand OXY E 404



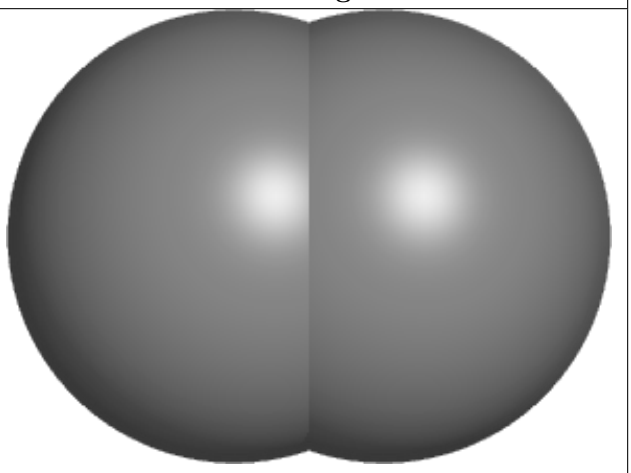
Bond lengths



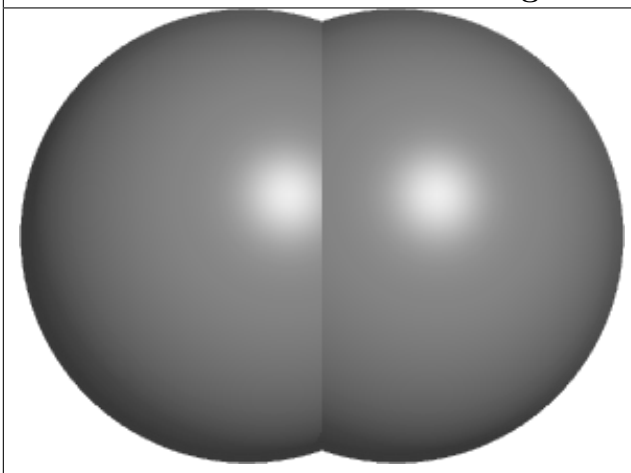
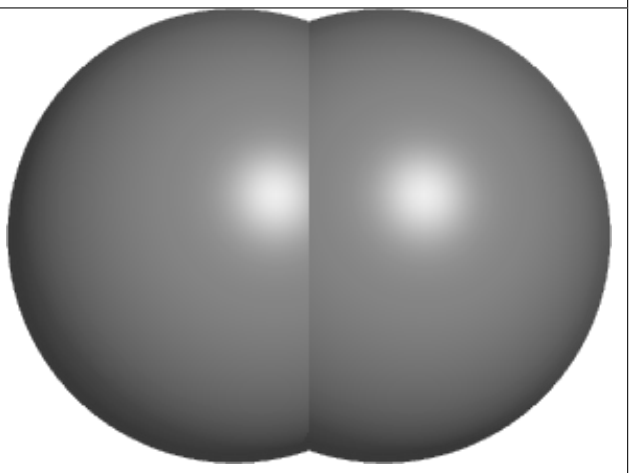
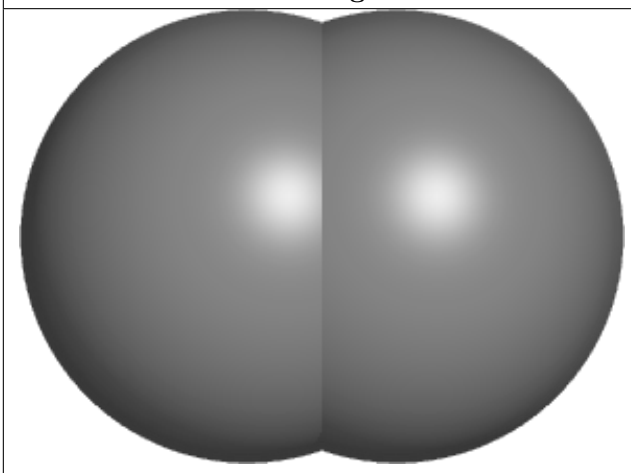
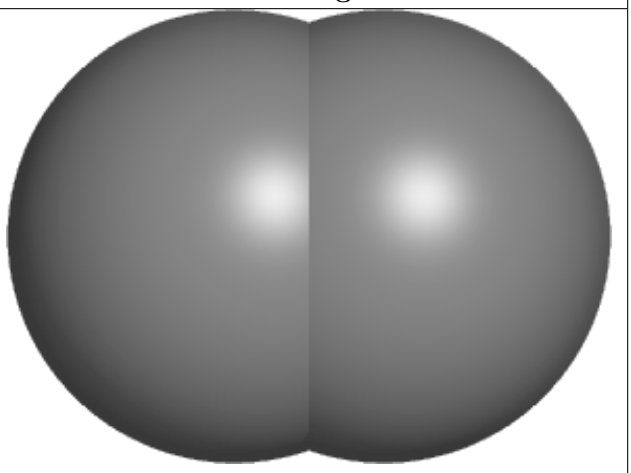
Bond angles



Torsions



Rings

Ligand OXY C 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

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

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, 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	A	278/283 (98%)	-0.04	11 (3%)	38	45	27, 34, 49, 78	1 (0%)
1	B	277/283 (97%)	0.03	10 (3%)	42	49	28, 37, 54, 92	0
1	C	277/283 (97%)	-0.19	5 (1%)	68	76	28, 36, 52, 63	1 (0%)
1	D	279/283 (98%)	0.07	11 (3%)	39	45	27, 37, 54, 76	0
1	E	277/283 (97%)	-0.08	8 (2%)	51	57	30, 38, 56, 91	1 (0%)
1	F	277/283 (97%)	-0.10	8 (2%)	51	57	27, 35, 52, 92	2 (0%)
All	All	1665/1698 (98%)	-0.05	53 (3%)	47	54	27, 36, 54, 92	5 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	40	ALA	7.5
1	A	40	ALA	6.0
1	F	316	ASP	5.4
1	A	231	TYR	4.2
1	E	316	ASP	3.9
1	A	263	ILE	3.7
1	E	40	ALA	3.4
1	B	263	ILE	3.4
1	B	316	ASP	3.3
1	A	230	TYR	3.2
1	A	267	ALA	3.2
1	C	120[A]	LYS	3.1
1	B	231	TYR	3.1
1	E	119	ASN	3.0
1	F	208	THR	3.0
1	D	41	GLY	2.9
1	F	230	TYR	2.9
1	A	316	ASP	2.8
1	A	226	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	231	TYR	2.8
1	E	312	ILE	2.8
1	B	259	ILE	2.7
1	A	228	GLY	2.7
1	D	230	TYR	2.7
1	B	233	THR	2.7
1	C	231	TYR	2.6
1	C	266	PRO	2.6
1	A	266	PRO	2.6
1	D	263	ILE	2.5
1	B	291	VAL	2.5
1	E	230	TYR	2.5
1	D	118	GLN	2.5
1	B	308	PRO	2.5
1	E	313	PRO	2.5
1	F	264	CYS	2.5
1	E	263	ILE	2.4
1	F	263	ILE	2.4
1	C	142	ALA	2.4
1	D	231	TYR	2.4
1	D	51	ARG	2.4
1	A	314	GLY	2.4
1	E	92	PHE	2.3
1	F	207	HIS	2.3
1	D	291	VAL	2.2
1	C	263	ILE	2.2
1	B	230	TYR	2.2
1	D	264	CYS	2.2
1	A	264	CYS	2.2
1	F	314	GLY	2.2
1	D	119	ASN	2.1
1	B	264	CYS	2.1
1	B	310	GLY	2.0
1	D	68	LEU	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)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.