Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2022 – 06:45 pm BST

PDB ID	:	7QR6
Title	:	Stilbene dioxygenase (NOV1) from Novosphingobium aromaticivorans: Ser283Phe mutant
Authors	:	Alvigini, L.; Mattevi, A.
Deposited on	:	2022-01-10
Resolution	:	2.90 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

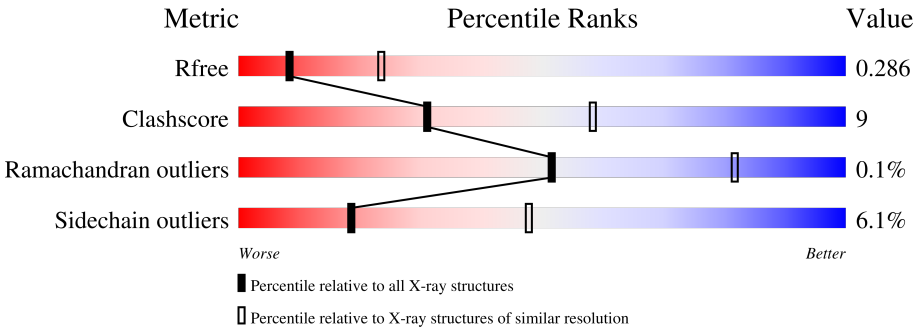
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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%

Mol	Chain	Length	Quality of chain
1	A	494	81% 14% 5%
1	B	494	78% 17%
1	C	494	68% 26%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11370 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 Dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	1	0
			3760	2397	648	690	25			
1	B	476	Total	C	N	O	S	0	1	0
			3795	2418	654	698	25			
1	C	475	Total	C	N	O	S	0	1	0
			3791	2418	654	694	25			

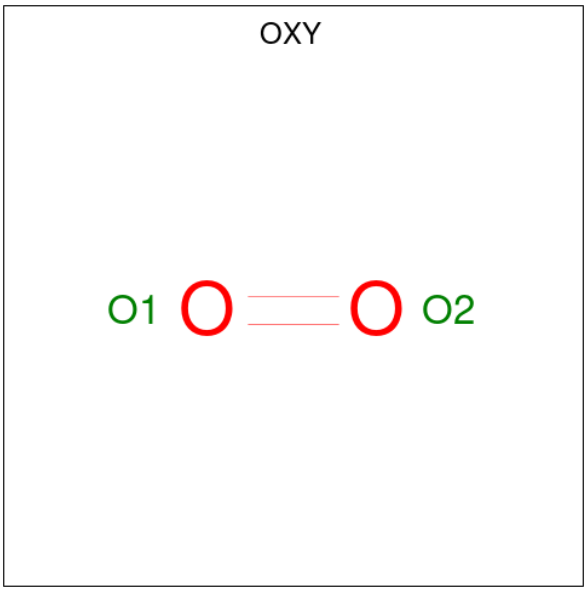
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	PHE	SER	conflict	UNP Q2GA76
B	283	PHE	SER	conflict	UNP Q2GA76
C	283	PHE	SER	conflict	UNP Q2GA76

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 2 2	0	0
3	B	1	Total O 2 2	0	0
3	C	1	Total O 2 2	0	0

- Molecule 4 is water.

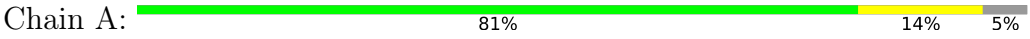
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	6	Total O 6 6	0	0
4	C	2	Total O 2 2	0	0

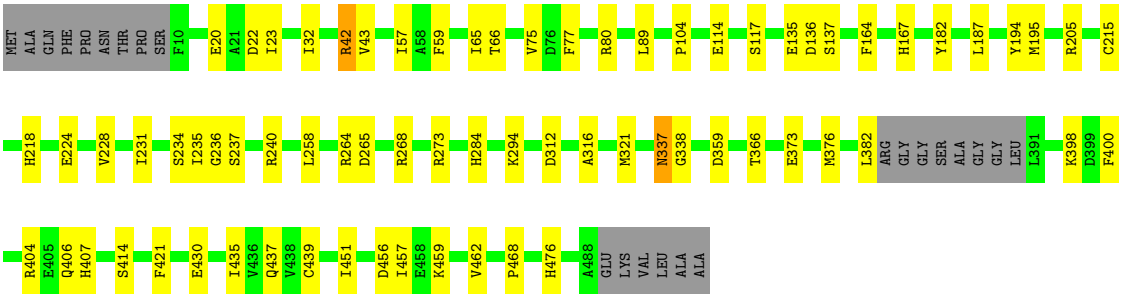
3 Residue-property plots (i)

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. 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. 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: Dioxygenase

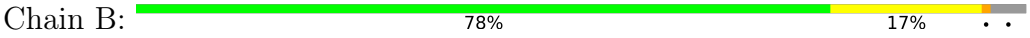
Chain A:

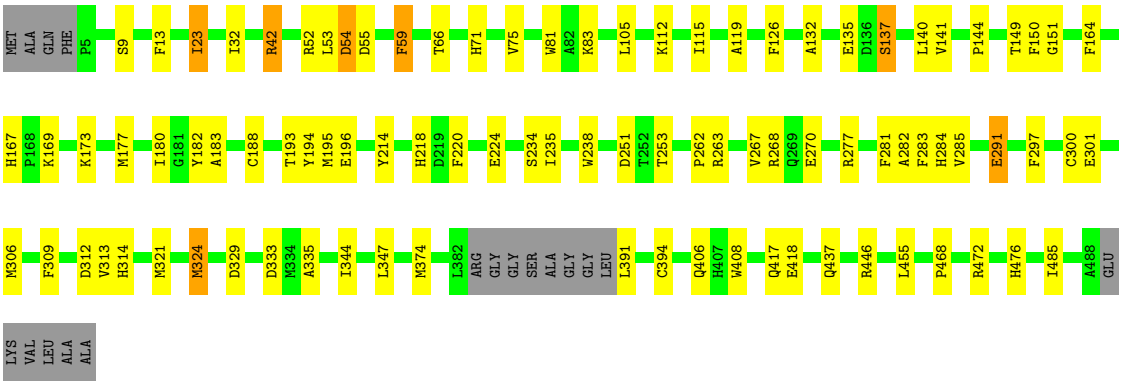




- Molecule 1: Dioxygenase

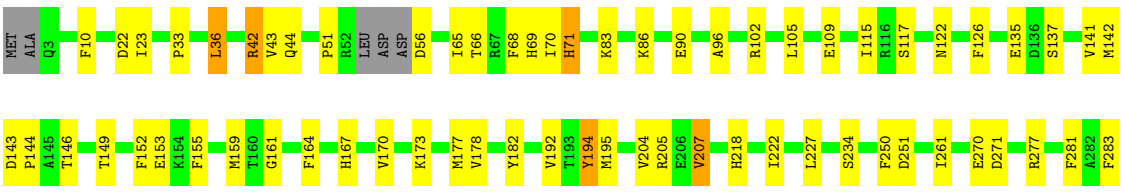
Chain B:

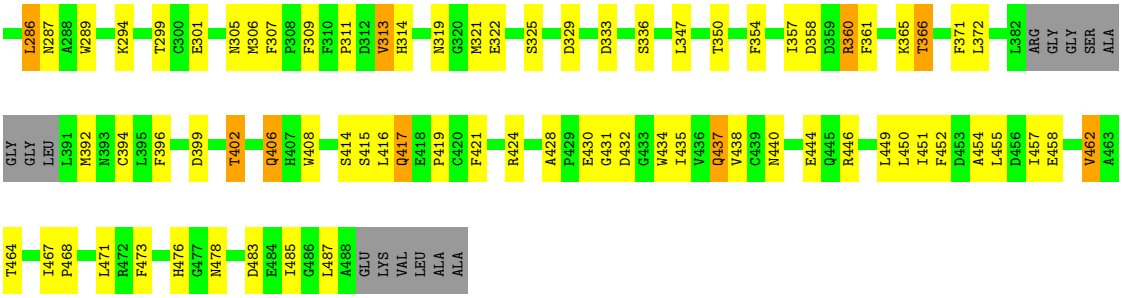




- Molecule 1: Dioxygenase

Chain C:




L286 N287 A288 W289 K294 T299 C300 E301 N305 M306 F307 P308 F309 F310 P311 D312 V313 H314 N319 G320 M321 E322 S325 D329 D333 S336 L347 T350 F354 I357 D358 D359 R360 F361 K365 T366 F371 L372 L382 ARG GLY GLY SER ALA
GLY GLY LEU L391 M392 N393 C394 L395 F396 D399 T402 Q406 H407 W408 S414 S415 L416 Q417 E418 P419 C420 F421 R424 A428 P429 E430 G431 D432 G433 W434 I435 V436 Q437 V438 C439 N440 E444 Q445 R446 L449 L450 I451 F452 D453 A454 L455 D456 I457 E458 V462 A463
T464 I467 P468 L471 R472 F473 H476 G477 N478 D483 E484 I485 G486 L487 A488 GLU LYS VAL LEU ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	178.47Å 187.98Å 105.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.90 48.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.04-2.90) 91.2 (48.99-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.214 , 0.291 0.218 , 0.286	Depositor DCC
R_{free} test set	1698 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.090	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	0.001 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11370	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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, FE

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	0.65	0/3874	0.83	1/5255 (0.0%)
1	B	0.64	0/3911	0.82	0/5307
1	C	0.64	0/3907	0.81	0/5300
All	All	0.65	0/11692	0.82	1/15862 (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	A	359	ASP	CB-CA-C	-6.70	96.99	110.40

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	3760	0	3575	35	0
1	B	3795	0	3608	57	0
1	C	3791	0	3604	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	7	0	0	0	0
4	B	6	0	0	0	0
4	C	2	0	0	0	0
All	All	11370	0	10787	201	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 9.

All (201) 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:53:LEU:HD23	1:B:54:ASP:H	1.04	1.09
1:C:144:PRO:CB	1:C:485:ILE:HG22	1.82	1.09
1:C:144:PRO:HB2	1:C:485:ILE:HG22	1.40	1.02
1:B:53:LEU:HD23	1:B:54:ASP:N	1.76	1.00
1:B:53:LEU:CD2	1:B:55:ASP:H	1.88	0.87
1:C:358:ASP:OD1	1:C:360:ARG:HG2	1.75	0.87
1:B:53:LEU:CD2	1:B:54:ASP:H	1.88	0.84
1:C:144:PRO:HB2	1:C:485:ILE:CG2	2.08	0.83
1:B:53:LEU:HD23	1:B:55:ASP:H	1.45	0.81
1:C:86:LYS:O	1:C:90:GLU:HG3	1.81	0.80
1:C:144:PRO:HB3	1:C:485:ILE:HG22	1.64	0.80
1:C:122:ASN:HD21	1:C:478:ASN:HD21	1.27	0.79
1:C:360:ARG:NH2	1:C:428:ALA:O	2.17	0.78
1:C:399:ASP:OD2	1:C:402:THR:CG2	2.33	0.76
1:C:361:PHE:CD2	1:C:430:GLU:HG3	2.22	0.75
1:C:69:HIS:HE1	1:C:71:HIS:ND1	1.87	0.72
1:C:33:PRO:HB2	1:C:36:LEU:HD12	1.71	0.72
1:A:312:ASP:OD2	1:A:316:ALA:HB3	1.91	0.71
1:C:153:GLU:OE2	1:C:155:PHE:N	2.21	0.69
1:A:337:ASN:HD22	1:A:337:ASN:N	1.92	0.67
1:C:286:LEU:CD1	1:C:357:ILE:CG2	2.72	0.66
1:A:42:ARG:HD3	1:A:66:THR:HB	1.77	0.66
1:C:281:PHE:CD2	1:C:305:ASN:HA	2.31	0.65
1:B:196:GLU:OE2	1:B:263:ARG:NH2	2.29	0.65
1:C:361:PHE:HE2	1:C:430:GLU:HA	1.62	0.64
1:C:277:ARG:NH1	1:C:301:GLU:OE1	2.29	0.64
1:C:286:LEU:HD12	1:C:357:ILE:CG2	2.28	0.64
1:A:23:ILE:HD13	1:A:468:PRO:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:GLU:O	1:B:291:GLU:HG2	1.98	0.63
1:A:23:ILE:HD13	1:A:468:PRO:CG	2.29	0.63
1:C:289:TRP:CE3	1:C:365:LYS:HA	2.33	0.63
1:C:286:LEU:HD12	1:C:357:ILE:HG23	1.81	0.63
1:B:53:LEU:HD23	1:B:55:ASP:N	2.12	0.62
1:C:399:ASP:OD2	1:C:402:THR:HG23	1.99	0.62
1:C:431:GLY:O	1:C:455:LEU:HD21	2.00	0.62
1:A:20:GLU:HG2	1:A:80:ARG:HA	1.82	0.62
1:C:319:ASN:ND2	1:C:322:GLU:CD	2.53	0.62
1:A:273:ARG:NH2	1:A:338:GLY:O	2.34	0.61
1:C:117:SER:HB2	1:C:137:SER:HB2	1.83	0.61
1:B:53:LEU:CD2	1:B:55:ASP:N	2.61	0.60
1:B:262:PRO:O	1:B:267:VAL:HG21	2.00	0.60
1:C:319:ASN:ND2	1:C:322:GLU:CG	2.65	0.59
1:C:250:PHE:O	1:C:313:VAL:HG22	2.03	0.59
1:C:286:LEU:HD11	1:C:357:ILE:HG22	1.82	0.59
1:C:358:ASP:OD1	1:C:360:ARG:CG	2.49	0.59
1:C:286:LEU:CD1	1:C:357:ILE:HG23	2.34	0.58
1:C:167:HIS:CD2	1:C:218:HIS:CE1	2.92	0.58
1:A:22:ASP:C	1:A:23:ILE:HG13	2.24	0.57
1:C:361:PHE:CE2	1:C:430:GLU:HA	2.39	0.57
1:A:22:ASP:O	1:A:23:ILE:HG13	2.05	0.57
1:C:454:ALA:O	1:C:457:ILE:HG23	2.05	0.57
1:B:251:ASP:OD1	1:B:253:THR:HB	2.05	0.56
1:B:406:GLN:NE2	1:B:455:LEU:O	2.38	0.56
1:C:69:HIS:HE1	1:C:71:HIS:CG	2.23	0.56
1:C:42:ARG:HD2	1:C:66:THR:HB	1.87	0.56
1:C:286:LEU:HD11	1:C:357:ILE:CG2	2.35	0.56
1:A:228:VAL:HG12	1:A:258:LEU:HD11	1.87	0.55
1:A:451:ILE:O	1:A:462:VAL:HG22	2.06	0.55
1:C:450:LEU:HD22	1:C:464:THR:HG23	1.87	0.54
1:C:69:HIS:HE1	1:C:71:HIS:CE1	2.25	0.54
1:A:32:ILE:HD13	1:A:75:VAL:HG23	1.90	0.54
1:C:167:HIS:CE1	1:C:476:HIS:CD2	2.91	0.54
1:C:182:TYR:HA	1:C:192:VAL:HG22	1.90	0.54
1:C:281:PHE:CE2	1:C:305:ASN:OD1	2.61	0.54
1:B:268:ARG:NE	1:B:270:GLU:OE2	2.41	0.54
1:C:319:ASN:HD21	1:C:322:GLU:HG3	1.73	0.53
1:C:23:ILE:CD1	1:C:468:PRO:HG2	2.39	0.53
1:B:42:ARG:HD2	1:B:66:THR:HB	1.90	0.53
1:C:83:LYS:HB2	1:C:149:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ILE:HD13	1:B:468:PRO:CG	2.38	0.53
1:C:178:VAL:HG11	1:C:222:ILE:HG21	1.91	0.53
1:B:83:LYS:HB2	1:B:149:THR:HG21	1.91	0.52
1:B:42:ARG:CD	1:B:66:THR:HB	2.41	0.51
1:C:434:TRP:HB3	1:C:452:PHE:O	2.10	0.51
1:C:329:ASP:HB2	1:C:347:LEU:HD21	1.93	0.51
1:B:188:CYS:HA	1:B:214:TYR:CE2	2.46	0.51
1:C:90:GLU:OE2	1:C:96:ALA:HA	2.10	0.50
1:B:235:ILE:HD12	1:B:235:ILE:C	2.32	0.50
1:A:456:ASP:O	1:A:459:LYS:HG2	2.11	0.50
1:A:421:PHE:HA	1:A:435:ILE:HD13	1.94	0.50
1:B:218:HIS:CD2	1:B:283:PHE:CZ	2.99	0.50
1:C:33:PRO:HB2	1:C:36:LEU:CD1	2.40	0.50
1:B:140:LEU:HD12	1:B:151:GLY:C	2.31	0.49
1:C:361:PHE:CE2	1:C:430:GLU:HB2	2.47	0.49
1:C:431:GLY:O	1:C:455:LEU:CD2	2.60	0.49
1:C:366:THR:HG22	1:C:430:GLU:CD	2.32	0.49
1:B:277:ARG:NH1	1:B:301:GLU:OE1	2.38	0.49
1:C:361:PHE:CE2	1:C:430:GLU:CB	2.95	0.49
1:B:32:ILE:HD13	1:B:75:VAL:HG23	1.94	0.49
1:C:69:HIS:CE1	1:C:71:HIS:CG	3.00	0.49
1:C:142:MET:HG2	1:C:149:THR:HA	1.94	0.49
1:B:183:ALA:HB2	1:B:214:TYR:HE2	1.78	0.49
1:C:417:GLN:HG3	1:C:438:VAL:O	2.12	0.49
1:A:373:GLU:OE1	1:A:407:HIS:ND1	2.45	0.48
1:A:89:LEU:HD11	1:A:114:GLU:OE1	2.14	0.48
1:C:287:ASN:ND2	1:C:366:THR:OG1	2.46	0.48
1:C:218:HIS:CD2	1:C:283:PHE:CZ	3.01	0.48
1:C:361:PHE:CE2	1:C:430:GLU:CA	2.96	0.48
1:A:167:HIS:CD2	1:A:218:HIS:CE1	3.02	0.48
1:C:227:LEU:HD23	1:C:261:ILE:HD13	1.95	0.48
1:C:143:ASP:HB3	1:C:146:THR:OG1	2.13	0.48
1:C:350:THR:HG21	1:C:396:PHE:CE2	2.49	0.47
1:C:309:PHE:O	1:C:311:PRO:HD3	2.14	0.47
1:B:119:ALA:HB1	1:B:132:ALA:HB1	1.96	0.47
1:B:169:LYS:HE2	1:B:220:PHE:O	2.15	0.47
1:B:374:MET:HG3	1:B:391:LEU:O	2.14	0.47
1:A:237:SER:OG	1:A:240:ARG:HG3	2.15	0.47
1:C:406:GLN:NE2	1:C:455:LEU:O	2.41	0.47
1:A:117:SER:HB2	1:A:137:SER:CB	2.45	0.47
1:A:236:GLY:HA2	1:A:240:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ARG:NH1	1:C:44:GLN:HB3	2.29	0.47
1:C:68:PHE:O	1:C:70:ILE:HG13	2.14	0.47
1:B:141:VAL:HG23	1:B:150:PHE:HB2	1.96	0.47
1:C:135:GLU:HA	1:C:164:PHE:O	2.15	0.47
1:C:406:GLN:HG2	1:C:458:GLU:HB3	1.96	0.47
1:C:251:ASP:OD1	1:C:314:HIS:HE1	1.98	0.47
1:C:358:ASP:OD1	1:C:360:ARG:CD	2.64	0.46
1:C:399:ASP:OD2	1:C:402:THR:HG22	2.14	0.46
1:B:417:GLN:O	1:B:437:GLN:NE2	2.48	0.46
1:A:398:LYS:HG2	1:A:400:PHE:CE1	2.50	0.46
1:A:136:ASP:OD1	1:A:137:SER:OG	2.31	0.46
1:C:167:HIS:HD2	1:C:218:HIS:CE1	2.34	0.46
1:C:361:PHE:CD2	1:C:430:GLU:CG	2.96	0.46
1:C:416:LEU:HD22	1:C:437:GLN:OE1	2.16	0.46
1:B:188:CYS:HA	1:B:214:TYR:CD2	2.51	0.46
1:C:319:ASN:ND2	1:C:322:GLU:HG3	2.28	0.46
1:A:366:THR:HB	1:A:430:GLU:OE2	2.16	0.46
1:B:23:ILE:HD13	1:B:468:PRO:HG3	1.96	0.46
1:B:282:ALA:HA	1:B:300:CYS:O	2.15	0.46
1:C:350:THR:HG21	1:C:396:PHE:CD2	2.51	0.46
1:B:81:TRP:HB2	1:B:83:LYS:HE2	1.97	0.45
1:B:115:ILE:HG23	1:B:137:SER:HB3	1.98	0.45
1:C:319:ASN:HD21	1:C:322:GLU:CG	2.28	0.45
1:C:218:HIS:CD2	1:C:283:PHE:CE1	3.05	0.45
1:B:312:ASP:OD1	1:B:314:HIS:N	2.46	0.45
1:B:281:PHE:CD1	1:B:306:MET:HG3	2.52	0.45
1:B:313:VAL:HG23	1:B:314:HIS:ND1	2.32	0.45
1:A:43:VAL:HG23	1:A:65:ILE:HD13	1.99	0.45
1:B:23:ILE:CD1	1:B:468:PRO:HG2	2.47	0.45
1:B:291:GLU:O	1:B:291:GLU:CG	2.65	0.45
1:C:227:LEU:CD2	1:C:261:ILE:HD13	2.47	0.45
1:C:117:SER:HB2	1:C:137:SER:CB	2.46	0.45
1:C:195:MET:HA	1:C:205:ARG:O	2.17	0.45
1:C:83:LYS:HB2	1:C:149:THR:CB	2.47	0.44
1:B:105:LEU:HD23	1:B:105:LEU:N	2.32	0.44
1:A:195:MET:HA	1:A:205:ARG:O	2.18	0.44
1:C:451:ILE:O	1:C:462:VAL:HG22	2.17	0.44
1:C:68:PHE:CD2	1:C:449:LEU:HD22	2.52	0.44
1:B:53:LEU:CD2	1:B:54:ASP:N	2.62	0.43
1:A:235:ILE:C	1:A:235:ILE:HD12	2.38	0.43
1:B:144:PRO:HB2	1:B:485:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASP:HB2	1:B:347:LEU:HD21	2.00	0.43
1:C:294:LYS:HE3	1:C:333:ASP:OD2	2.17	0.43
1:A:167:HIS:CE1	1:A:284:HIS:CD2	3.07	0.43
1:B:126:PHE:CD2	1:B:177:MET:CE	3.00	0.43
1:A:406:GLN:OE1	1:A:457:ILE:N	2.52	0.43
1:C:42:ARG:HH12	1:C:44:GLN:HB3	1.84	0.43
1:A:135:GLU:HA	1:A:164:PHE:O	2.18	0.43
1:B:126:PHE:CD2	1:B:177:MET:HE3	2.54	0.43
1:C:421:PHE:HA	1:C:435:ILE:HD13	2.00	0.43
1:C:115:ILE:HG21	1:C:152:PHE:CE2	2.54	0.42
1:A:104:PRO:HG2	1:A:187:LEU:HD22	2.00	0.42
1:C:43:VAL:HG23	1:C:65:ILE:HD13	2.01	0.42
1:C:467:ILE:HD13	1:C:471:LEU:HD11	2.01	0.42
1:B:23:ILE:HD13	1:B:468:PRO:HG2	2.00	0.42
1:B:253:THR:HG22	1:B:253:THR:O	2.19	0.42
1:B:167:HIS:CE1	1:B:284:HIS:CD2	3.08	0.42
1:B:418:GLU:OE2	1:B:476:HIS:ND1	2.47	0.42
1:C:10:PHE:CZ	1:C:51:PRO:HG3	2.54	0.42
1:B:135:GLU:HA	1:B:164:PHE:O	2.19	0.42
1:C:126:PHE:CD2	1:C:177:MET:CE	3.03	0.42
1:B:324:MET:HE2	1:B:324:MET:HA	2.02	0.42
1:B:333:ASP:OD1	1:B:335:ALA:HB3	2.20	0.42
1:C:43:VAL:HG23	1:C:65:ILE:CD1	2.50	0.41
1:B:135:GLU:OE2	1:B:182:TYR:OH	2.32	0.41
1:C:23:ILE:CD1	1:C:468:PRO:CG	2.98	0.41
1:C:33:PRO:O	1:C:36:LEU:HD12	2.19	0.41
1:B:285:VAL:HG22	1:B:297:PHE:CZ	2.56	0.41
1:C:218:HIS:HD2	1:C:283:PHE:CE1	2.38	0.41
1:C:414:SER:HA	1:C:440:ASN:O	2.19	0.41
1:C:283:PHE:CZ	1:C:307:PHE:HZ	2.38	0.41
1:A:136:ASP:OD1	1:A:136:ASP:C	2.58	0.41
1:C:419:PRO:HA	1:C:437:GLN:HB3	2.02	0.41
1:B:173:LYS:NZ	1:B:224:GLU:OE2	2.43	0.41
1:A:312:ASP:OD2	1:A:316:ALA:CB	2.66	0.41
1:A:23:ILE:HD12	1:A:77:PHE:CD1	2.55	0.41
1:C:394:CYS:HA	1:C:408:TRP:O	2.21	0.41
1:A:215:CYS:SG	1:A:231:ILE:HG23	2.61	0.41
1:C:159:MET:CE	1:C:161:GLY:O	2.69	0.41
1:C:424[B]:ARG:NE	1:C:432:ASP:OD2	2.54	0.41
1:B:180:ILE:HA	1:B:193:THR:O	2.21	0.41
1:C:173:LYS:HD3	1:C:173:LYS:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:PRO:CB	1:C:485:ILE:CG2	2.71	0.40
1:C:354:PHE:CD2	1:C:372:LEU:HD12	2.56	0.40
1:C:69:HIS:CD2	1:C:487:LEU:HD13	2.56	0.40
1:C:286:LEU:HD22	1:C:371:PHE:CE2	2.56	0.40
1:A:167:HIS:CE1	1:A:476:HIS:CD2	3.07	0.40
1:B:394:CYS:HA	1:B:408:TRP:O	2.21	0.40
1:C:271:ASP:OD1	1:C:271:ASP:N	2.53	0.40
1:C:194:TYR:CD2	1:C:207:VAL:CG2	3.05	0.40
1:C:281:PHE:CD1	1:C:306:MET:HG3	2.56	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	468/494 (95%)	445 (95%)	22 (5%)	1 (0%)	47 78
1	B	473/494 (96%)	445 (94%)	27 (6%)	1 (0%)	47 78
1	C	470/494 (95%)	442 (94%)	28 (6%)	0	100 100
All	All	1411/1482 (95%)	1332 (94%)	77 (6%)	2 (0%)	51 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	PHE
1	A	59	PHE

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	395/409 (97%)	377 (95%)	18 (5%)	27	60
1	B	400/409 (98%)	379 (95%)	21 (5%)	22	54
1	C	399/409 (98%)	365 (92%)	34 (8%)	10	31
All	All	1194/1227 (97%)	1121 (94%)	73 (6%)	18	48

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	57	ILE
1	A	182	TYR
1	A	194	TYR
1	A	224	GLU
1	A	234	SER
1	A	264	ARG
1	A	265	ASP
1	A	268	ARG
1	A	294	LYS
1	A	321	MET
1	A	337	ASN
1	A	376	MET
1	A	382	LEU
1	A	404	ARG
1	A	414	SER
1	A	437	GLN
1	A	439	CYS
1	B	9	SER
1	B	13	PHE
1	B	23	ILE
1	B	42	ARG
1	B	52	ARG
1	B	54	ASP
1	B	59	PHE
1	B	71	HIS
1	B	112	LYS
1	B	137	SER
1	B	194	TYR
1	B	195	MET

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Mol	Chain	Res	Type
1	B	234	SER
1	B	238	TRP
1	B	291	GLU
1	B	309	PHE
1	B	321	MET
1	B	324	MET
1	B	344	ILE
1	B	446	ARG
1	B	472	ARG
1	C	22	ASP
1	C	36	LEU
1	C	42	ARG
1	C	56	ASP
1	C	71	HIS
1	C	102	ARG
1	C	105	LEU
1	C	109	GLU
1	C	141	VAL
1	C	170	VAL
1	C	194	TYR
1	C	204	VAL
1	C	207	VAL
1	C	234	SER
1	C	270	GLU
1	C	286	LEU
1	C	299	THR
1	C	313	VAL
1	C	321	MET
1	C	325	SER
1	C	336	SER
1	C	360	ARG
1	C	366	THR
1	C	392	MET
1	C	402	THR
1	C	406	GLN
1	C	415	SER
1	C	417	GLN
1	C	437	GLN
1	C	444	GLU
1	C	446	ARG
1	C	462	VAL
1	C	473	PHE

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Mol	Chain	Res	Type
1	C	483	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	69	HIS
1	A	91	ASN
1	A	337	ASN
1	B	48	GLN
1	B	69	HIS
1	B	91	ASN
1	B	466	ASN
1	C	69	HIS
1	C	314	HIS
1	C	466	ASN
1	C	478	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	OXY	C	502	2	1,1,1	0.19	0	-		
3	OXY	A	502	2	1,1,1	0.17	0	-		
3	OXY	B	502	2	1,1,1	0.11	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.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

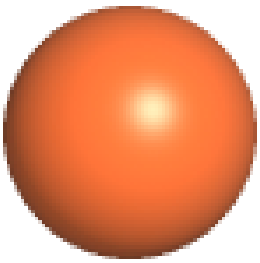
6.4 Ligands

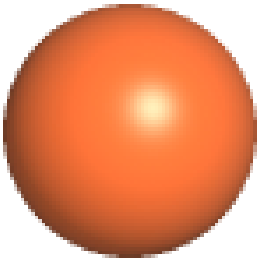
Unable to reproduce the depositors R factor - this section is therefore empty.

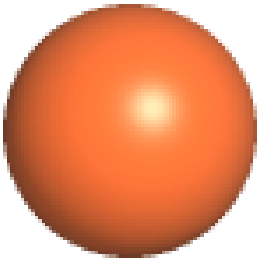
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FE A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

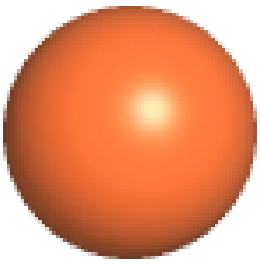


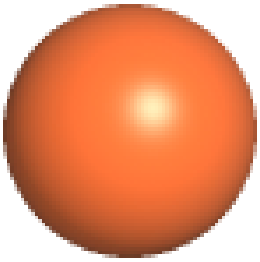


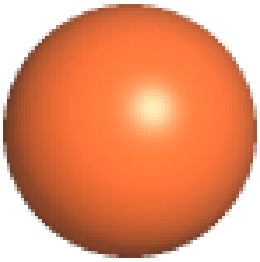


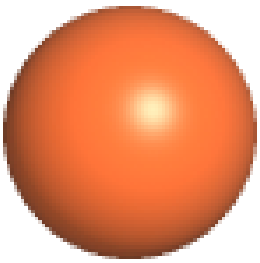
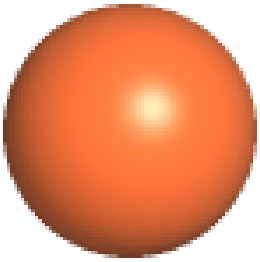
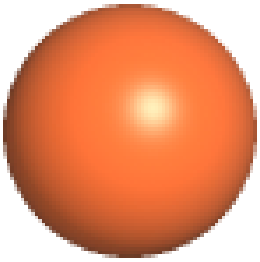
Electron density around FE B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around FE C 501: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.