Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 05:39 PM JST

PDB ID	:	5GN7
Title	:	Crystal structure of alternative oxidase from Trypanosoma brucei brucei complexed with cumarin derivative-17
Authors	:	Balogun, E.O.; Inaoka, D.K.; Shiba, T.; Tsuge, T.; May, B.; Sato, T.; Kido, Y.; Takeshi, N.; Aoki, T.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Michels, P.A.M.; Watanabe, Y.; Moore, A.L.; Harada, S.; Kita, K.
Deposited on	:	2016-07-19
Resolution	:	3.20 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:

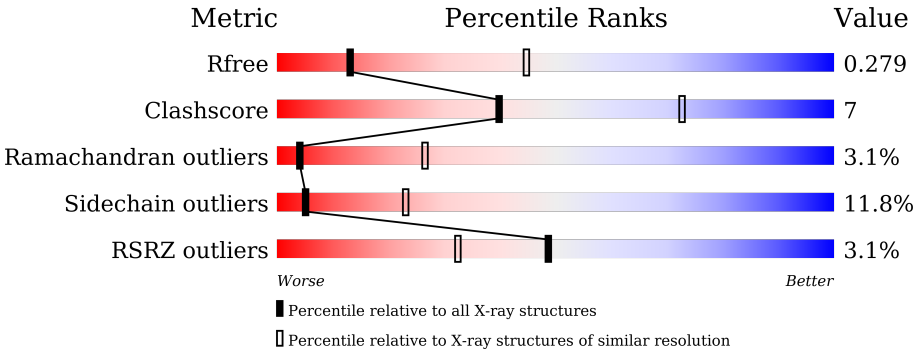
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	329	56% 21% • 20%
1	B	329	53% 23% • 20%
1	C	329	61% 18% • 20%
1	D	329	55% 23% • 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8623 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.

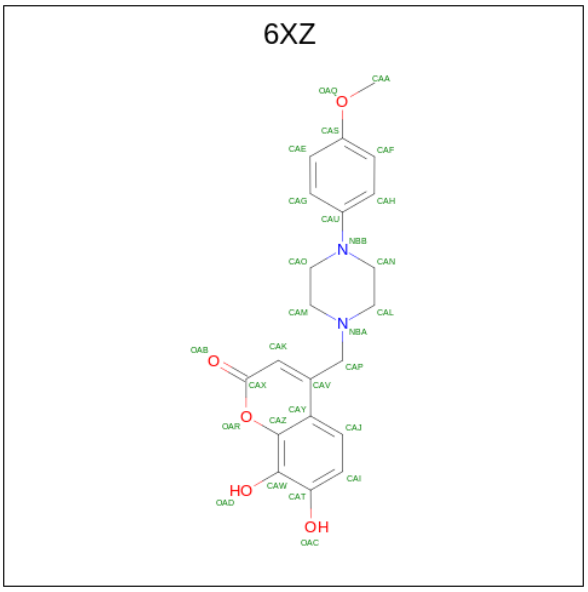
- Molecule 1 is a protein called Alternative oxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2146	1375	381	380	10			
1	B	264	Total	C	N	O	S	0	0	0
			2146	1375	381	380	10			
1	C	264	Total	C	N	O	S	0	0	0
			2146	1375	381	380	10			
1	D	264	Total	C	N	O	S	0	0	0
			2146	1375	381	380	10			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

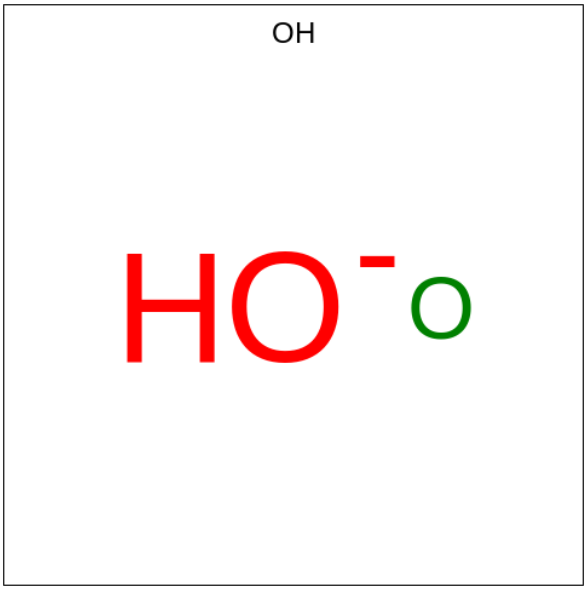
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		

- Molecule 3 is 4-[[4-(4-methoxyphenyl)piperazin-1-yl]methyl]-7,8-bis(oxidanyl)chromen-2-one (three-letter code: 6XZ) (formula: $C_{21}H_{22}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	21	2	5		

- Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



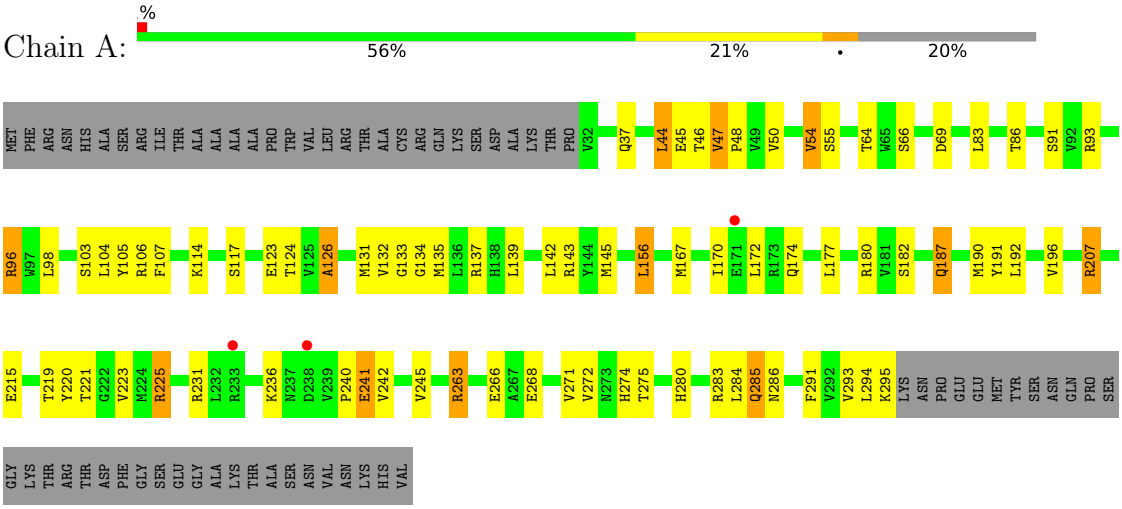
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O		0	0
			1	1			
4	C	1	Total	O		0	0
			1	1			
4	D	1	Total	O		0	0
			1	1			

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.

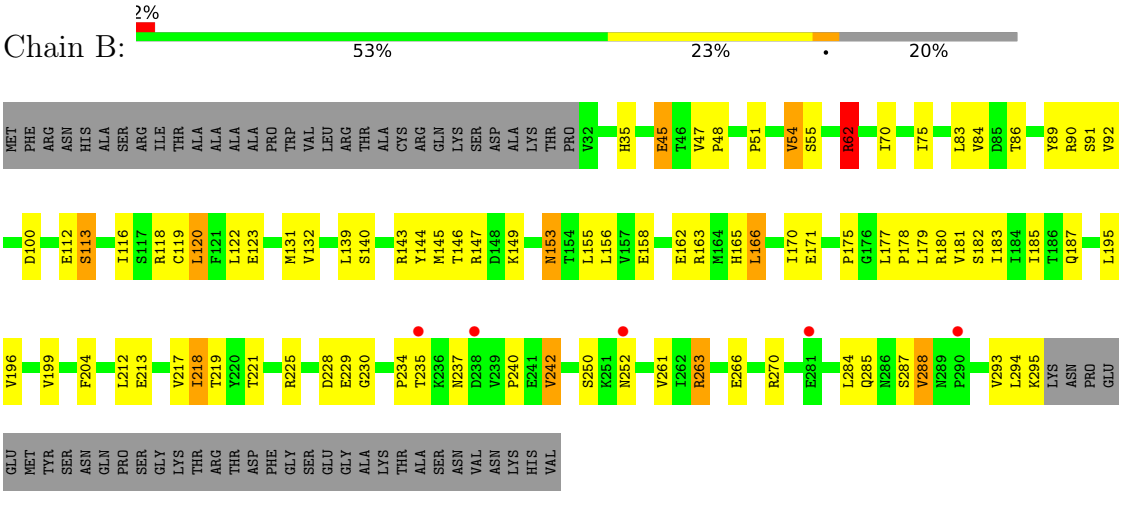
• Molecule 1: Alternative oxidase, mitochondrial

Chain A:



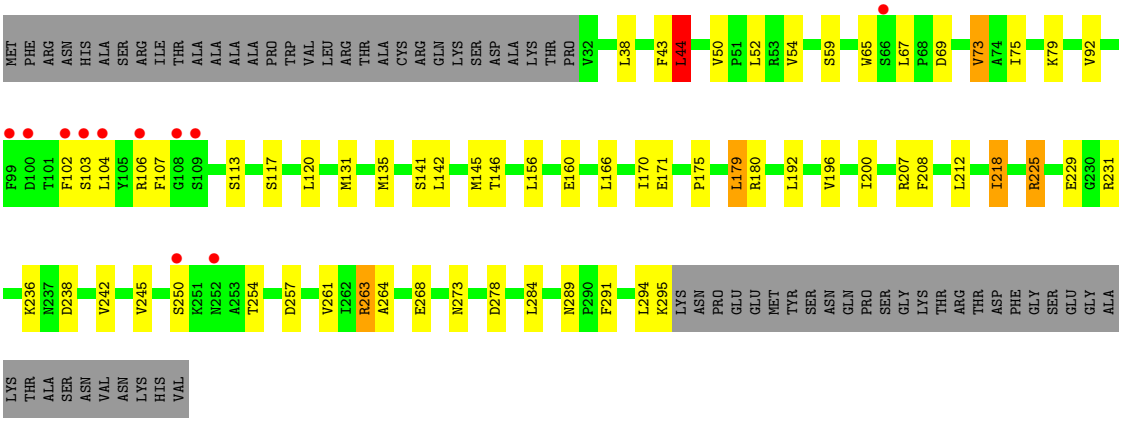
• Molecule 1: Alternative oxidase, mitochondrial

Chain B:



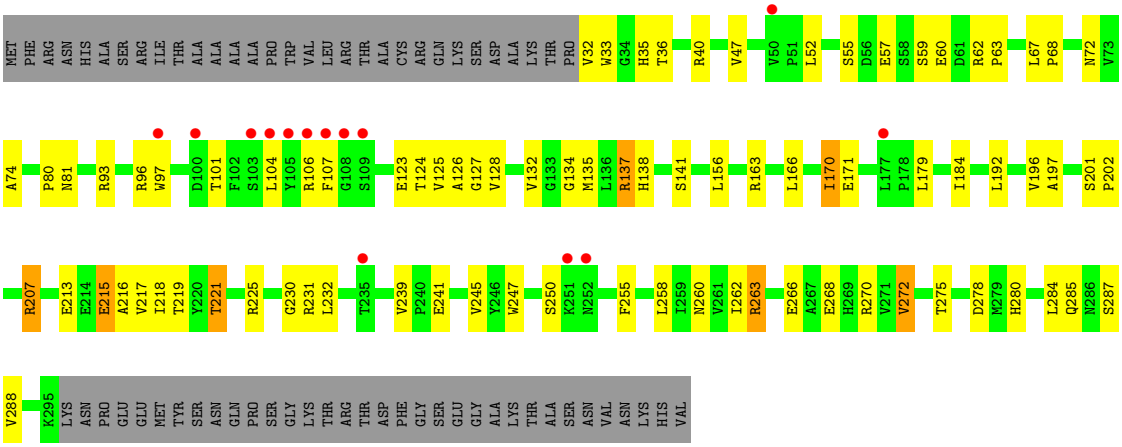
• Molecule 1: Alternative oxidase, mitochondrial

Chain C:



• Molecule 1: Alternative oxidase, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.31Å 222.73Å 63.16Å 90.00° 114.70° 90.00°	Depositor
Resolution (Å)	45.54 – 3.20 45.54 – 3.20	Depositor EDS
% Data completeness (in resolution range)	86.5 (45.54-3.20) 92.3 (45.54-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.195 , 0.268 0.206 , 0.279	Depositor DCC
R_{free} test set	1468 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	80.5	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.199 for -h-2*l,-k,l	Xtriage
Reported twinning fraction	0.557 for H, K, L 0.443 for H+4/2L, -K, -L	Depositor
Outliers	1 of 28859 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8623	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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: OH, FE, 6XZ

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	0.67	0/2195	0.94	5/2982 (0.2%)
1	B	0.69	0/2195	0.93	1/2982 (0.0%)
1	C	0.63	0/2195	0.88	0/2982
1	D	0.66	0/2195	0.87	4/2982 (0.1%)
All	All	0.66	0/8780	0.91	10/11928 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	225	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	143	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	207	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	166	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	137	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	D	137	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	137	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	207	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	D	40	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	62	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	2146	0	2175	40	0
1	B	2146	0	2175	48	0
1	C	2146	0	2175	26	0
1	D	2146	0	2175	34	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	28	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	8623	0	8700	126	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 7.

All (126) 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:A:221:THR:HG22	1:A:263:ARG:HE	1.48	0.76
1:B:54:VAL:HG22	1:B:242:VAL:HG13	1.75	0.69
1:C:69:ASP:OD1	1:D:35:HIS:ND1	2.22	0.68
1:A:293:VAL:O	1:A:295:LYS:N	2.28	0.66
1:B:221:THR:CG2	1:B:263:ARG:HE	2.08	0.66
1:A:93:ARG:NH2	1:A:215:GLU:OE2	2.34	0.61
1:C:131:MET:HG3	1:D:135:MET:HG2	1.83	0.59
1:B:234:PRO:O	1:B:237:ASN:ND2	2.35	0.59
1:D:213:GLU:HA	1:D:213:GLU:OE1	2.03	0.58
1:C:254:THR:N	1:C:257:ASP:OD2	2.36	0.58
1:D:272:VAL:O	1:D:275:THR:N	2.37	0.57
1:B:217:VAL:HG13	1:B:263:ARG:HD3	1.87	0.57
1:C:175:PRO:HB3	1:C:179:LEU:HD12	1.85	0.57
1:D:217:VAL:O	1:D:221:THR:OG1	2.23	0.56
1:A:54:VAL:HG13	1:A:242:VAL:HA	1.87	0.56
1:D:215:GLU:O	1:D:218:ILE:N	2.38	0.56
1:D:55:SER:O	1:D:62:ARG:NH2	2.39	0.56
1:A:191:TYR:CE2	1:B:139:LEU:HD11	2.42	0.55
1:D:97:TRP:CH2	1:D:101:THR:HG21	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:MET:HG2	1:B:131:MET:HG3	1.89	0.55
1:A:268:GLU:O	1:A:271:VAL:HG22	2.07	0.55
1:B:100:ASP:OD1	1:B:118:ARG:NH2	2.38	0.55
1:A:123:GLU:HA	1:A:126:ALA:HB3	1.88	0.54
1:A:167:MET:HE2	1:B:147:ARG:HA	1.88	0.54
1:B:92:VAL:HG13	1:B:212:LEU:HD23	1.90	0.54
1:C:75:ILE:HD11	1:C:218:ILE:HA	1.89	0.54
1:B:293:VAL:O	1:B:295:LYS:N	2.41	0.54
1:A:135:MET:O	1:A:139:LEU:HG	2.08	0.53
1:C:261:VAL:O	1:C:264:ALA:N	2.41	0.53
1:C:142:LEU:HD11	1:D:127:GLY:O	2.08	0.53
1:B:90:ARG:NH1	1:C:229:GLU:O	2.43	0.52
1:C:207:ARG:NH1	1:C:278:ASP:OD1	2.34	0.51
1:B:119:CYS:O	1:B:123:GLU:HG2	2.11	0.51
1:A:191:TYR:CD2	1:B:139:LEU:HD11	2.45	0.51
1:C:273:ASN:N	1:C:273:ASN:OD1	2.44	0.51
1:A:187:GLN:NE2	1:B:143:ARG:HB3	2.26	0.51
1:C:268:GLU:OE2	1:D:33:TRP:NE1	2.44	0.50
1:A:190:MET:O	1:A:191:TYR:C	2.50	0.49
1:D:239:VAL:HG13	1:D:258:LEU:HD22	1.93	0.49
1:B:179:LEU:HD13	1:B:183:ILE:HD12	1.94	0.49
1:A:69:ASP:OD1	1:B:35:HIS:ND1	2.41	0.49
1:D:197:ALA:O	1:D:201:SER:O	2.31	0.49
1:C:236:LYS:HE3	1:C:238:ASP:HB2	1.95	0.49
1:B:123:GLU:HB2	1:B:166:LEU:HB2	1.94	0.48
1:A:44:LEU:O	1:A:47:VAL:HG13	2.13	0.48
1:C:289:ASN:OD1	1:C:291:PHE:N	2.46	0.48
1:C:295:LYS:O	1:C:295:LYS:CG	2.61	0.48
1:D:134:GLY:HA3	1:D:156:LEU:HD13	1.96	0.48
1:A:220:TYR:CE2	1:A:266:GLU:HG3	2.49	0.47
1:D:230:GLY:O	1:D:232:LEU:N	2.48	0.47
1:B:75:ILE:HB	1:C:75:ILE:HB	1.96	0.47
1:B:89:TYR:OH	1:C:225:ARG:HG3	2.14	0.47
1:C:145:MET:HB3	1:D:170:ILE:HG13	1.96	0.47
1:B:45:GLU:O	1:B:48:PRO:HD2	2.15	0.47
1:D:217:VAL:HG11	1:D:270:ARG:HH12	1.80	0.47
1:A:44:LEU:O	1:A:44:LEU:HD22	2.15	0.46
1:A:145:MET:SD	1:B:120:LEU:HD11	2.55	0.46
1:D:60:GLU:OE1	1:D:62:ARG:NH1	2.48	0.46
1:B:153:ASN:OD1	1:B:153:ASN:C	2.54	0.46
1:B:177:LEU:O	1:B:178:PRO:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HB3	1:B:187:GLN:NE2	2.31	0.46
1:B:181:VAL:O	1:B:182:SER:C	2.55	0.46
1:B:112:GLU:HG2	1:B:116:ILE:HD13	1.99	0.45
1:A:134:GLY:HA3	1:A:156:LEU:HD13	1.98	0.45
1:B:55:SER:O	1:B:62:ARG:NH2	2.49	0.45
1:B:123:GLU:OE1	1:B:162:GLU:OE1	2.35	0.45
1:A:220:TYR:HE2	1:A:266:GLU:HG3	1.82	0.44
1:A:142:LEU:HD23	1:B:163:ARG:HG3	2.00	0.44
1:B:165:HIS:CE1	1:B:266:GLU:OE1	2.71	0.44
1:C:59:SER:N	1:C:160:GLU:OE2	2.44	0.44
1:D:74:ALA:O	1:D:270:ARG:NH2	2.48	0.44
1:D:207:ARG:NH2	1:D:278:ASP:OD1	2.43	0.44
1:D:262:ILE:O	1:D:266:GLU:HG2	2.18	0.44
1:B:221:THR:HG23	1:B:263:ARG:HE	1.82	0.44
1:A:47:VAL:N	1:A:48:PRO:CD	2.81	0.44
1:A:219:THR:OG1	3:A:503:6XZ:OAB	2.25	0.43
1:B:149:LYS:HB3	1:B:288:VAL:HA	2.00	0.43
1:C:92:VAL:HG23	1:C:208:PHE:CD1	2.53	0.43
1:A:103:SER:O	1:A:105:TYR:N	2.51	0.43
1:B:70:ILE:CD1	1:B:261:VAL:HA	2.49	0.43
1:D:32:VAL:O	1:D:32:VAL:HG13	2.18	0.43
1:A:271:VAL:HG23	1:A:272:VAL:N	2.34	0.43
1:D:57:GLU:O	1:D:163:ARG:NH1	2.51	0.43
1:A:54:VAL:HG22	1:A:242:VAL:CG1	2.47	0.43
1:A:54:VAL:HG22	1:A:242:VAL:HG13	2.01	0.43
1:A:275:THR:HG21	1:A:291:PHE:CE2	2.53	0.43
1:A:96:ARG:NE	1:A:215:GLU:OE1	2.48	0.43
1:A:50:VAL:HG13	1:B:288:VAL:CG1	2.49	0.42
1:A:293:VAL:HG21	1:B:51:PRO:HD2	2.02	0.42
1:B:84:VAL:HG13	1:B:204:PHE:HB2	2.01	0.42
1:B:171:GLU:OE2	1:B:240:PRO:HB3	2.19	0.42
1:B:250:SER:OG	1:B:252:ASN:N	2.50	0.42
1:C:38:LEU:HD22	1:D:268:GLU:HA	2.01	0.42
1:C:73:VAL:HG11	1:C:263:ARG:HD3	2.00	0.42
1:D:202:PRO:HB2	1:D:280:HIS:CD2	2.53	0.42
1:A:131:MET:HB2	1:A:131:MET:HE2	1.85	0.42
1:A:54:VAL:HG12	1:A:245:VAL:HG21	2.02	0.42
1:B:54:VAL:CG2	1:B:242:VAL:HG13	2.47	0.42
1:D:221:THR:HG23	1:D:263:ARG:HE	1.85	0.42
1:A:207:ARG:HH11	1:A:274:HIS:HD2	1.68	0.42
1:B:195:LEU:O	1:B:199:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PHE:O	1:C:44:LEU:C	2.57	0.42
1:C:50:VAL:HG13	1:D:288:VAL:CG1	2.50	0.42
1:D:63:PRO:HG2	1:D:247:TRP:CD1	2.54	0.42
1:D:67:LEU:HB2	1:D:68:PRO:HD3	2.00	0.42
1:D:192:LEU:O	1:D:196:VAL:HG12	2.20	0.42
1:D:215:GLU:O	1:D:216:ALA:C	2.58	0.42
1:D:218:ILE:O	1:D:219:THR:C	2.58	0.42
1:A:280:HIS:CD2	1:A:285:GLN:HG2	2.55	0.41
1:D:138:HIS:O	1:D:141:SER:HB3	2.20	0.41
1:A:240:PRO:O	1:A:241:GLU:C	2.58	0.41
1:B:144:TYR:O	1:B:146:THR:HG23	2.20	0.41
1:B:218:ILE:O	1:B:219:THR:C	2.57	0.41
1:C:141:SER:HA	1:C:146:THR:OG1	2.20	0.41
1:C:254:THR:OG1	1:C:257:ASP:OD2	2.36	0.41
1:A:172:LEU:O	1:A:236:LYS:NZ	2.44	0.41
1:B:228:ASP:O	1:B:230:GLY:N	2.54	0.41
1:D:123:GLU:O	1:D:126:ALA:N	2.54	0.41
1:A:280:HIS:O	1:A:283:ARG:N	2.50	0.41
1:B:213:GLU:HA	1:B:213:GLU:OE1	2.21	0.41
1:B:112:GLU:OE1	1:B:234:PRO:HA	2.21	0.41
1:A:145:MET:HG2	1:B:166:LEU:HD21	2.01	0.40
1:B:120:LEU:HD21	1:B:175:PRO:HB3	2.03	0.40
1:C:236:LYS:HG2	1:C:238:ASP:HB2	2.04	0.40
1:D:123:GLU:O	1:D:125:VAL:N	2.54	0.40
1:B:123:GLU:OE1	1:B:165:HIS:ND1	2.49	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	262/329 (80%)	226 (86%)	26 (10%)	10 (4%)	3 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	262/329 (80%)	215 (82%)	40 (15%)	7 (3%)	5 30
1	C	262/329 (80%)	227 (87%)	28 (11%)	7 (3%)	5 30
1	D	262/329 (80%)	217 (83%)	36 (14%)	9 (3%)	3 24
All	All	1048/1316 (80%)	885 (84%)	130 (12%)	33 (3%)	4 26

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	294	LEU
1	D	231	ARG
1	D	287	SER
1	A	156	LEU
1	A	223	VAL
1	B	218	ILE
1	B	229	GLU
1	B	294	LEU
1	C	44	LEU
1	C	120	LEU
1	C	200	ILE
1	A	104	LEU
1	A	126	ALA
1	A	241	GLU
1	B	120	LEU
1	B	145	MET
1	C	113	SER
1	D	215	GLU
1	D	255	PHE
1	D	272	VAL
1	A	133	GLY
1	A	231	ARG
1	B	270	ARG
1	C	73	VAL
1	C	103	SER
1	D	124	THR
1	B	113	SER
1	D	128	VAL
1	D	250	SER
1	C	218	ILE
1	D	80	PRO
1	A	177	LEU

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	239/292 (82%)	208 (87%)	31 (13%)	4	19
1	B	239/292 (82%)	211 (88%)	28 (12%)	5	23
1	C	239/292 (82%)	210 (88%)	29 (12%)	5	22
1	D	239/292 (82%)	214 (90%)	25 (10%)	7	28
All	All	956/1168 (82%)	843 (88%)	113 (12%)	5	23

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	44	LEU
1	A	45	GLU
1	A	46	THR
1	A	47	VAL
1	A	55	SER
1	A	64	THR
1	A	66	SER
1	A	83	LEU
1	A	86	THR
1	A	91	SER
1	A	96	ARG
1	A	98	LEU
1	A	106	ARG
1	A	107	PHE
1	A	114	LYS
1	A	117	SER
1	A	124	THR
1	A	132	VAL
1	A	170	ILE
1	A	174	GLN
1	A	180	ARG
1	A	182	SER
1	A	187	GLN

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Mol	Chain	Res	Type
1	A	192	LEU
1	A	196	VAL
1	A	225	ARG
1	A	263	ARG
1	A	284	LEU
1	A	285	GLN
1	A	286	ASN
1	B	45	GLU
1	B	47	VAL
1	B	54	VAL
1	B	62	ARG
1	B	83	LEU
1	B	86	THR
1	B	91	SER
1	B	113	SER
1	B	122	LEU
1	B	132	VAL
1	B	140	SER
1	B	153	ASN
1	B	155	LEU
1	B	156	LEU
1	B	158	GLU
1	B	166	LEU
1	B	170	ILE
1	B	180	ARG
1	B	185	ILE
1	B	196	VAL
1	B	225	ARG
1	B	235	THR
1	B	242	VAL
1	B	263	ARG
1	B	284	LEU
1	B	285	GLN
1	B	287	SER
1	B	288	VAL
1	C	44	LEU
1	C	52	LEU
1	C	54	VAL
1	C	65	TRP
1	C	67	LEU
1	C	79	LYS
1	C	102	PHE

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Mol	Chain	Res	Type
1	C	104	LEU
1	C	106	ARG
1	C	107	PHE
1	C	117	SER
1	C	135	MET
1	C	156	LEU
1	C	166	LEU
1	C	170	ILE
1	C	171	GLU
1	C	179	LEU
1	C	180	ARG
1	C	192	LEU
1	C	196	VAL
1	C	212	LEU
1	C	225	ARG
1	C	231	ARG
1	C	242	VAL
1	C	245	VAL
1	C	250	SER
1	C	263	ARG
1	C	284	LEU
1	C	294	LEU
1	D	36	THR
1	D	47	VAL
1	D	52	LEU
1	D	59	SER
1	D	72	ASN
1	D	81	ASN
1	D	93	ARG
1	D	96	ARG
1	D	104	LEU
1	D	106	ARG
1	D	107	PHE
1	D	132	VAL
1	D	137	ARG
1	D	170	ILE
1	D	171	GLU
1	D	179	LEU
1	D	184	ILE
1	D	221	THR
1	D	225	ARG
1	D	241	GLU

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Mol	Chain	Res	Type
1	D	245	VAL
1	D	260	ASN
1	D	263	ARG
1	D	284	LEU
1	D	285	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	252	ASN
1	A	273	ASN
1	A	274	HIS
1	A	286	ASN
1	B	81	ASN
1	B	187	GLN
1	B	252	ASN
1	B	260	ASN
1	B	273	ASN
1	B	274	HIS
1	B	285	GLN
1	C	81	ASN
1	C	187	GLN
1	C	248	ASN
1	D	77	HIS
1	D	165	HIS
1	D	248	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 (i)

Of 12 ligands modelled in this entry, 8 are monoatomic and 3 are modelled with single atom - leaving 1 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	6XZ	A	503	2	31,31,31	1.68	4 (12%)	43,44,44	2.42	14 (32%)

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
3	6XZ	A	503	2	-	4/10/20/20	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	6XZ	CAP-CAV	-5.49	1.44	1.50
3	A	503	6XZ	CAO-NBB	3.41	1.52	1.46
3	A	503	6XZ	CAW-CAZ	3.09	1.44	1.39
3	A	503	6XZ	CAK-CAX	-2.68	1.38	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	6XZ	OAB-CAX-CAK	-6.35	112.88	125.84
3	A	503	6XZ	CAP-CAV-CAY	6.10	127.10	118.19
3	A	503	6XZ	OAR-CAX-OAB	6.10	124.21	116.44
3	A	503	6XZ	OAR-CAX-CAK	4.36	122.79	117.17
3	A	503	6XZ	CAZ-OAR-CAX	-3.65	118.87	121.99
3	A	503	6XZ	CAP-NBA-CAM	3.56	116.61	111.09
3	A	503	6XZ	CAM-CAO-NBB	3.53	117.55	110.70
3	A	503	6XZ	CAP-NBA-CAL	-3.03	106.40	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	6XZ	CAP-CAV-CAK	-3.03	115.05	121.59
3	A	503	6XZ	CAE-CAG-CAU	2.74	123.93	120.32
3	A	503	6XZ	CAH-CAU-NBB	2.65	125.03	121.38
3	A	503	6XZ	OAR-CAZ-CAW	2.32	120.10	116.42
3	A	503	6XZ	OAR-CAZ-CAY	-2.16	118.69	121.27
3	A	503	6XZ	CAG-CAU-NBB	-2.03	118.58	121.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	6XZ	CAE-CAS-OAQ-CAA
3	A	503	6XZ	CAF-CAS-OAQ-CAA
3	A	503	6XZ	NBA-CAP-CAV-CAY
3	A	503	6XZ	NBA-CAP-CAV-CAK

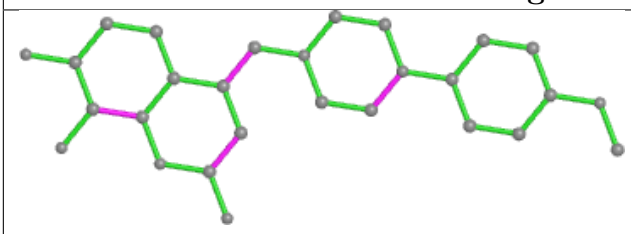
There are no ring outliers.

1 monomer is involved in 1 short contact:

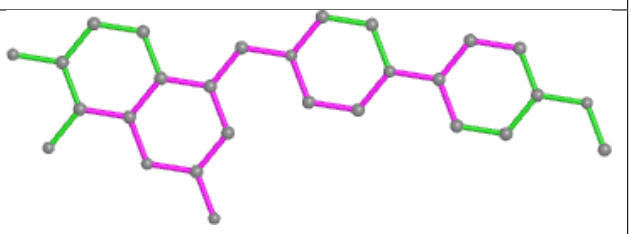
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	6XZ	1	0

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.

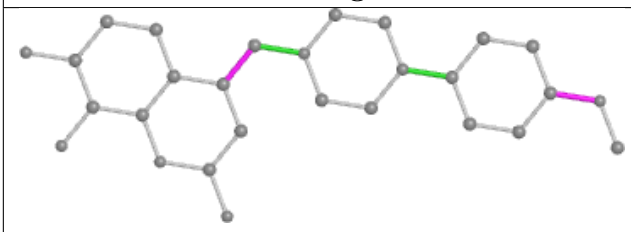
Ligand 6XZ A 503



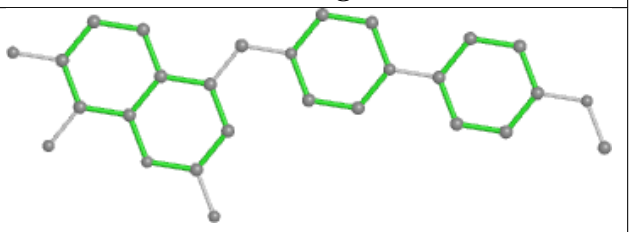
Bond lengths



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	264/329 (80%)	-0.21	3 (1%)	80	69	37, 63, 101, 133	0
1	B	264/329 (80%)	-0.20	5 (1%)	66	53	42, 65, 95, 122	0
1	C	264/329 (80%)	0.13	11 (4%)	36	23	47, 81, 146, 202	0
1	D	264/329 (80%)	0.06	14 (5%)	26	14	46, 79, 128, 170	0
All	All	1056/1316 (80%)	-0.05	33 (3%)	49	32	37, 72, 122, 202	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	SER	7.9
1	C	103	SER	5.4
1	D	109	SER	3.9
1	D	105	TYR	3.8
1	C	104	LEU	3.8
1	C	100	ASP	3.7
1	C	252	ASN	3.4
1	D	106	ARG	3.3
1	D	103	SER	3.3
1	C	102	PHE	3.2
1	C	108	GLY	3.0
1	C	106	ARG	3.0
1	A	238	ASP	2.9
1	C	66	SER	2.9
1	D	252	ASN	2.8
1	D	97	TRP	2.8
1	D	107	PHE	2.7
1	D	104	LEU	2.7
1	A	233	ARG	2.6
1	B	290	PRO	2.5
1	D	251	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	108	GLY	2.4
1	A	171	GLU	2.3
1	B	235	THR	2.3
1	B	281	GLU	2.3
1	C	99	PHE	2.3
1	D	235	THR	2.3
1	C	250	SER	2.3
1	B	238	ASP	2.2
1	B	252	ASN	2.1
1	D	50	VAL	2.1
1	D	177	LEU	2.1
1	D	100	ASP	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
3	6XZ	A	503	28/28	0.90	0.27	61,97,118,125	0
2	FE	A	502	1/1	0.95	0.09	54,54,54,54	0
2	FE	D	502	1/1	0.97	0.10	50,50,50,50	0
2	FE	D	501	1/1	0.98	0.10	61,61,61,61	0
2	FE	B	501	1/1	0.98	0.07	57,57,57,57	0
2	FE	B	502	1/1	0.98	0.07	52,52,52,52	0
4	OH	C	503	1/1	0.98	0.12	59,59,59,59	0
2	FE	C	501	1/1	0.99	0.15	62,62,62,62	0
2	FE	C	502	1/1	0.99	0.11	66,66,66,66	0
4	OH	B	503	1/1	0.99	0.09	58,58,58,58	0
2	FE	A	501	1/1	0.99	0.09	57,57,57,57	0

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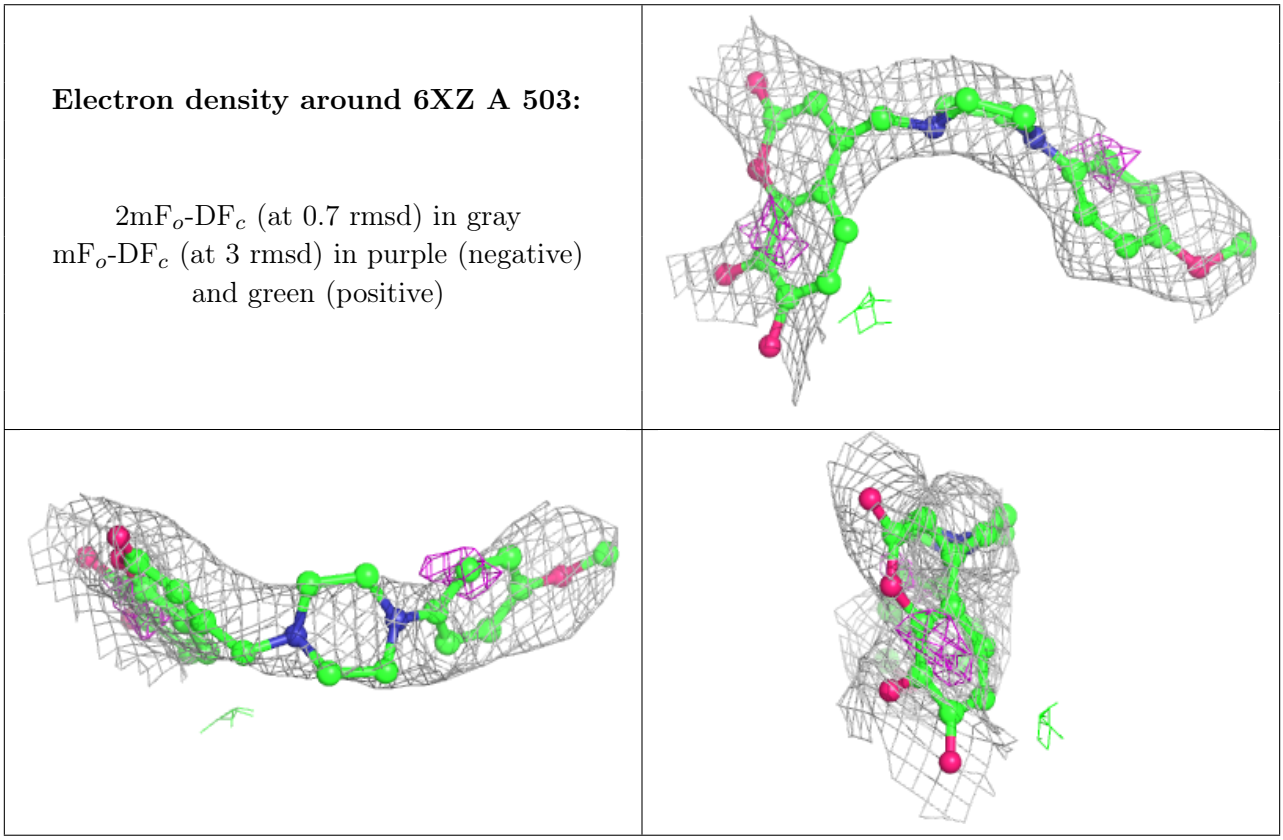
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OH	D	503	1/1	0.99	0.15	38,38,38,38	0

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.

Electron density around 6XZ A 503:

$2mF_o$-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)

There are no such residues in this entry.