



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:18 AM UTC

PDB ID : 5ZDP / pdb_00005zdp
Title : Crystal structure of cyanide-insensitive alternative oxidase from Trypanosoma brucei with ferulenol
Authors : Shiba, T.; Inaoka, D.K.; Takahashi, G.; Tsuge, C.; Kido, Y.; Young, L.; Ueda, S.; Balogun, E.O.; Nara, T.; Honma, T.; Tanaka, A.; Inoue, M.; Saimoto, H.; Harada, S.; Moore, A.L.; Kita, K.
Deposited on : 2018-02-23
Resolution : 2.71 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](#) ①) were used in the production of this report:

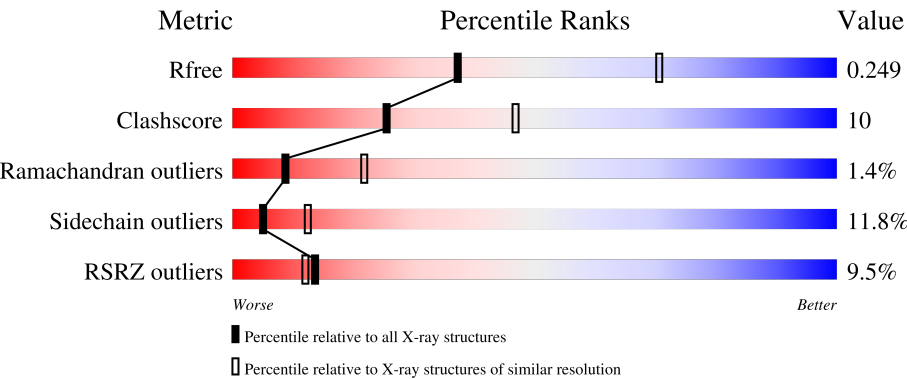
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.71 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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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 $\leq 5\%$. 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	4% 59% 19% .. 20%
1	B	329	5% 53% 22% .. 20%
1	C	329	9% 60% 17% .. 19%
1	D	329	12% 58% 18% . 19%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8796 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.

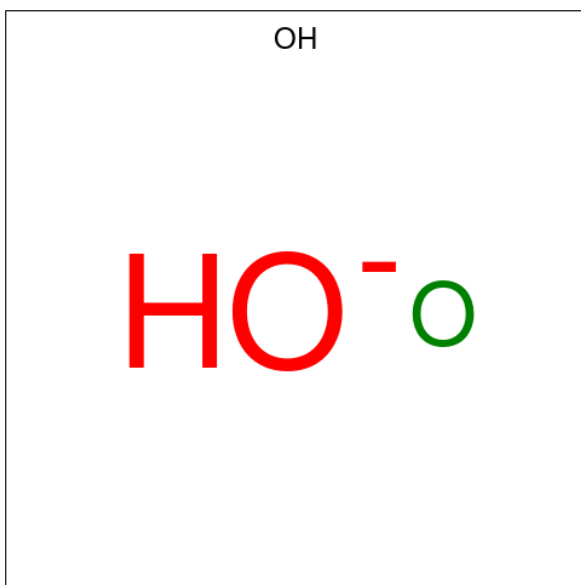
- Molecule 1 is a protein called Alternative oxidase, mitochondrial.

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	263	Total	C	N	O	S	0	0	0
			2137	1369	379	379	10			
1	C	266	Total	C	N	O	S	0	0	0
			2162	1386	384	382	10			
1	D	265	Total	C	N	O	S	0	0	0
			2153	1380	382	381	10			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

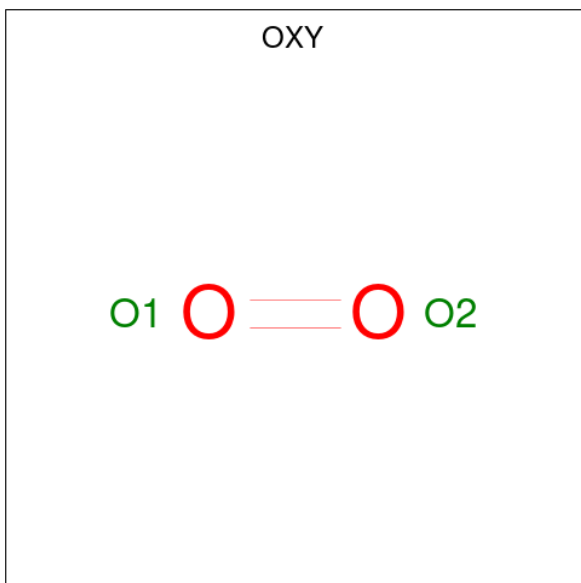
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		

- Molecule 3 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



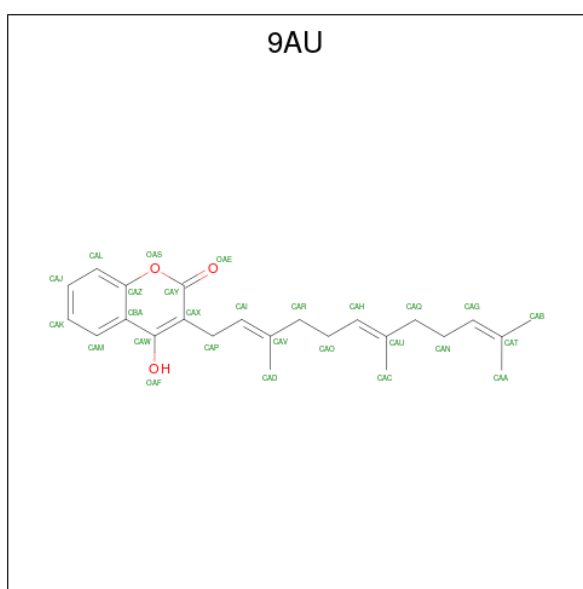
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 5 is 4-oxidanyl-3-[(2 {E},6 {E})-3,7,11-trimethyldodeca-2,6,10-trienyl]chromen-2-one (CCD ID: 9AU) (formula: $C_{24}H_{30}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 27	C 24	O 3	0	0
5	B	1	Total 27	C 24	O 3	0	0
5	C	1	Total 27	C 24	O 3	0	0
5	D	1	Total 27	C 24	O 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	23	Total O 23 23	0	0

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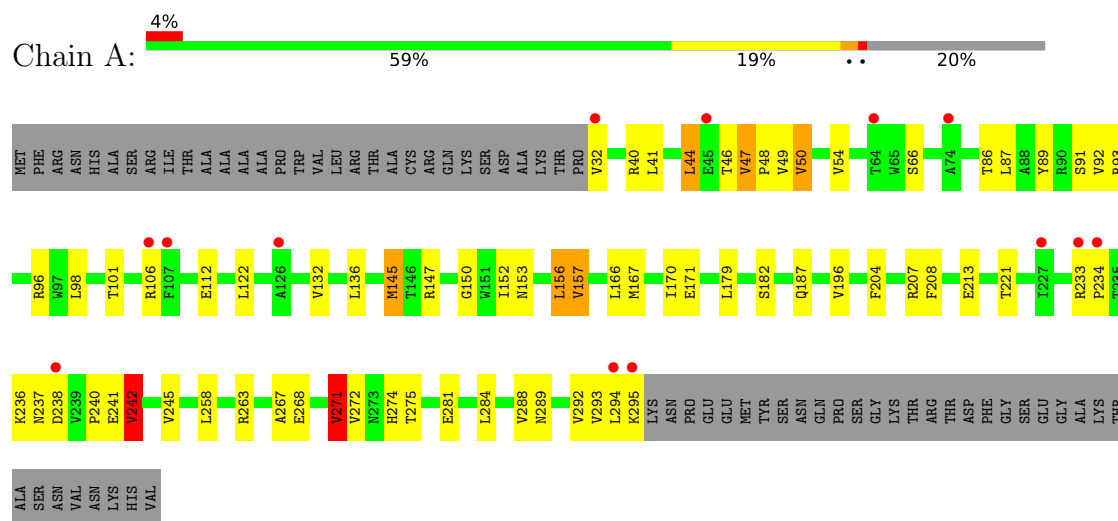
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	24	Total 24	O 24	0	0
6	C	14	Total 14	O 14	0	0
6	D	9	Total 9	O 9	0	0

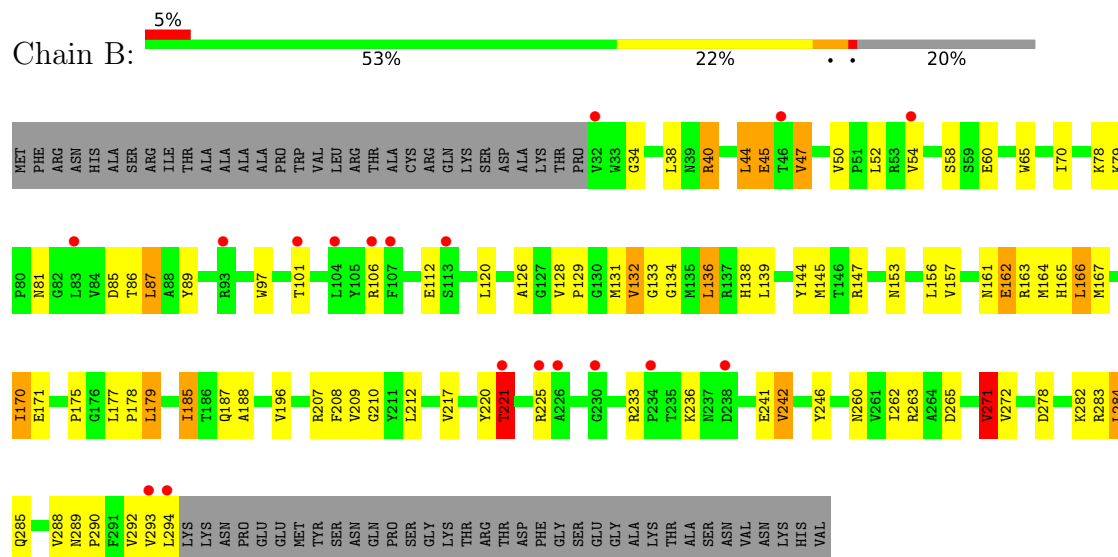
3 Residue-property plots

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

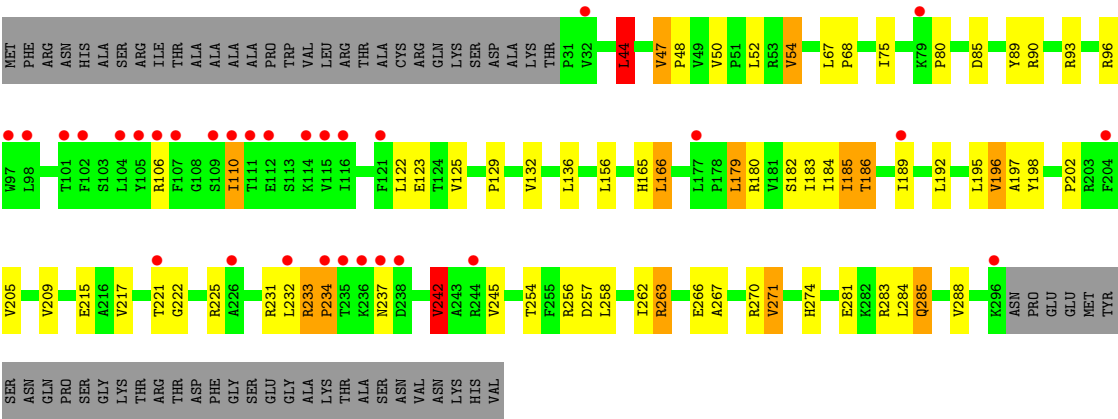


- Molecule 1: Alternative oxidase, mitochondrial

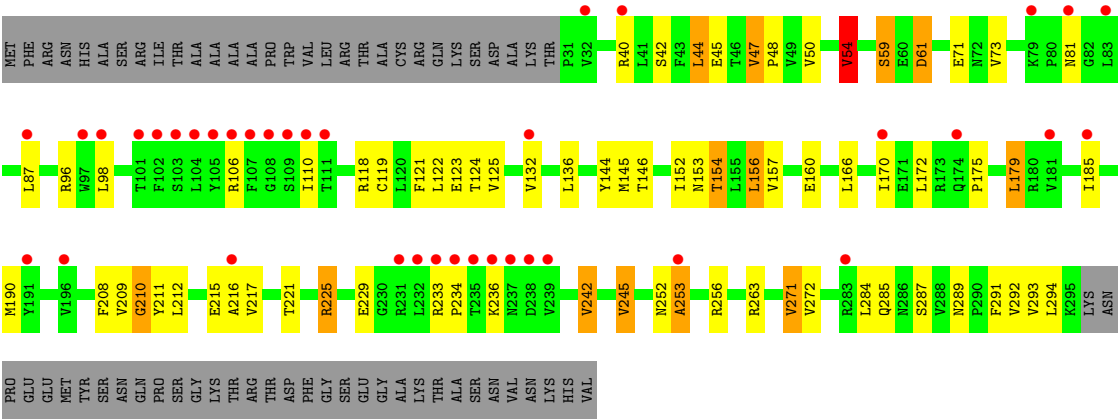


- Molecule 1: Alternative oxidase, mitochondrial





● Molecule 1: Alternative oxidase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	259.50Å 63.11Å 138.27Å 90.00° 122.21° 90.00°	Depositor
Resolution (Å)	39.32 – 2.71 39.32 – 2.71	Depositor EDS
% Data completeness (in resolution range)	92.6 (39.32-2.71) 95.0 (39.32-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.192 , 0.249 0.202 , 0.249	Depositor DCC
R_{free} test set	2582 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.216 for -h-2*1,-k,l	Xtriage
Reported twinning fraction	0.539 for H, K, L 0.461 for H+4/2L, -K, -L	Depositor
Outliers	0 of 49577 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8796	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, OXY, 9AU

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	0.69	0/2195	1.00	3/2982 (0.1%)
1	B	0.70	0/2186	0.98	4/2971 (0.1%)
1	C	0.75	0/2212	0.95	4/3004 (0.1%)
1	D	0.60	0/2203	0.87	1/2993 (0.0%)
All	All	0.69	0/8796	0.95	12/11950 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	242	VAL	CB-CA-C	-7.05	102.86	111.88
1	B	138	HIS	N-CA-C	-6.41	104.22	111.14
1	B	271	VAL	CB-CA-C	-6.39	103.63	111.87
1	C	271	VAL	CB-CA-C	-6.11	104.17	111.81
1	A	49	VAL	CA-C-N	-5.79	117.71	123.04
1	A	49	VAL	C-N-CA	-5.79	117.71	123.04
1	D	271	VAL	CB-CA-C	-5.67	104.71	111.97
1	B	162	GLU	N-CA-C	-5.59	105.19	111.28
1	B	221	THR	N-CA-CB	5.47	118.35	110.20
1	C	180	ARG	N-CA-C	-5.46	105.22	111.07
1	A	271	VAL	CB-CA-C	-5.40	104.85	112.14
1	C	184	ILE	N-CA-C	5.17	115.89	110.62

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	48	0
1	B	2137	0	2162	60	0
1	C	2162	0	2196	43	0
1	D	2153	0	2183	32	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	1	0	0	0	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	27	0	0	4	0
5	B	27	0	0	2	0
5	C	27	0	0	6	0
5	D	27	0	0	2	0
6	A	23	0	0	1	0
6	B	24	0	0	1	0
6	C	14	0	0	1	0
6	D	9	0	0	1	0
All	All	8796	0	8716	167	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 10.

All (167) 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:C:185:ILE:C	1:C:185:ILE:HD12	1.58	1.23
1:C:185:ILE:C	1:C:185:ILE:CD1	2.34	1.00
1:C:185:ILE:HD12	1:C:185:ILE:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:O	1:A:47:VAL:HG13	1.70	0.91
1:C:217:VAL:O	1:C:221:THR:HG22	1.74	0.87
1:C:75:ILE:HD11	1:C:221:THR:HG21	1.58	0.84
1:C:185:ILE:CD1	1:C:185:ILE:O	2.30	0.79
1:C:262:ILE:O	1:C:266:GLU:HG2	1.84	0.78
1:B:208:PHE:CE2	1:B:212:LEU:HD11	2.22	0.75
1:A:96:ARG:HA	5:A:505:9AU:CAD	2.18	0.72
1:B:289:ASN:O	1:B:292:VAL:HG22	1.91	0.71
1:A:221:THR:HG22	1:A:263:ARG:HH21	1.56	0.71
1:B:294:LEU:H	1:B:294:LEU:HD22	1.56	0.69
1:C:263:ARG:HD3	6:C:604:HOH:O	1.93	0.69
1:B:153:ASN:O	1:B:157:VAL:HG22	1.93	0.67
1:D:208:PHE:CE2	1:D:212:LEU:HD11	2.31	0.65
1:D:185:ILE:HD11	6:D:609:HOH:O	1.96	0.65
3:C:503:OH:O	5:C:505:9AU:CAK	2.46	0.64
1:A:236:LYS:O	1:A:238:ASP:N	2.31	0.63
1:C:185:ILE:HD12	1:C:186:THR:N	2.12	0.63
1:D:40:ARG:NH2	1:D:42:SER:O	2.31	0.63
1:B:112:GLU:OE2	1:B:236:LYS:HG2	1.99	0.62
1:C:123:GLU:OE2	1:C:123:GLU:HA	2.00	0.60
1:D:289:ASN:O	1:D:292:VAL:HG22	2.01	0.60
1:D:292:VAL:HG23	1:D:293:VAL:HG23	1.82	0.60
1:A:207:ARG:HD3	1:A:274:HIS:CD2	2.37	0.59
1:B:161:ASN:ND2	1:B:246:TYR:OH	2.30	0.58
1:B:217:VAL:O	1:B:221:THR:HG23	2.03	0.58
1:A:293:VAL:O	1:A:295:LYS:N	2.37	0.58
1:B:294:LEU:HD22	1:B:294:LEU:N	2.19	0.58
1:C:185:ILE:HD11	1:C:189:ILE:HD12	1.85	0.58
1:C:185:ILE:HD11	1:C:189:ILE:CD1	2.34	0.57
1:A:44:LEU:HG	1:B:278:ASP:HB3	1.87	0.57
5:A:505:9AU:CAI	5:A:505:9AU:OAF	2.52	0.57
1:A:145:MET:HB3	1:B:170:ILE:HG13	1.87	0.57
1:B:44:LEU:O	1:B:47:VAL:HG13	2.04	0.57
1:D:122:LEU:HD13	5:D:505:9AU:CAW	2.35	0.56
3:B:503:OH:O	5:B:505:9AU:CAK	2.54	0.56
1:A:147:ARG:HA	1:B:167:MET:CE	2.37	0.55
1:A:207:ARG:NH1	6:A:602:HOH:O	2.40	0.55
1:A:147:ARG:HA	1:B:167:MET:HE1	1.88	0.55
1:C:234:PRO:O	1:C:237:ASN:ND2	2.41	0.54
1:C:75:ILE:HD11	1:C:221:THR:CG2	2.33	0.54
1:A:293:VAL:C	1:A:295:LYS:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:TYR:OH	1:D:225:ARG:HG3	2.08	0.53
1:C:96:ARG:HA	5:C:505:9AU:CAD	2.38	0.53
1:C:166:LEU:HD22	1:C:166:LEU:O	2.10	0.53
1:C:44:LEU:O	1:C:44:LEU:HD22	2.10	0.52
1:A:47:VAL:HG12	1:B:290:PRO:HG3	1.92	0.52
1:B:207:ARG:O	1:B:208:PHE:C	2.51	0.51
1:C:258:LEU:C	1:C:258:LEU:HD23	2.35	0.51
1:B:65:TRP:HB3	1:B:70:ILE:HD13	1.93	0.51
1:A:147:ARG:HD3	1:B:167:MET:HE2	1.92	0.51
1:D:209:VAL:O	1:D:210:GLY:C	2.54	0.51
1:A:46:THR:O	1:A:50:VAL:HG13	2.12	0.50
1:D:121:PHE:O	1:D:124:THR:OG1	2.27	0.50
1:B:293:VAL:O	1:B:294:LEU:C	2.54	0.50
1:C:196:VAL:O	1:C:197:ALA:C	2.54	0.50
1:A:271:VAL:CG1	1:B:40:ARG:O	2.60	0.50
1:C:182:SER:O	1:C:186:THR:OG1	2.28	0.50
5:C:505:9AU:CAI	5:C:505:9AU:OAF	2.59	0.50
1:C:96:ARG:NH1	1:C:215:GLU:OE1	2.39	0.49
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.12	0.49
1:A:293:VAL:C	1:A:295:LYS:N	2.71	0.49
5:D:505:9AU:CAI	5:D:505:9AU:OAF	2.61	0.49
1:C:254:THR:OG1	1:C:257:ASP:OD1	2.27	0.48
1:A:147:ARG:CA	1:B:167:MET:HE1	2.44	0.48
1:D:47:VAL:O	1:D:50:VAL:HG12	2.13	0.48
1:C:233:ARG:O	1:C:234:PRO:C	2.57	0.48
1:A:156:LEU:HD11	1:B:131:MET:HE1	1.95	0.48
1:C:179:LEU:O	1:C:183:ILE:HD12	2.13	0.48
1:B:97:TRP:O	1:B:101:THR:HG23	2.15	0.47
1:D:125:VAL:HG13	1:D:190:MET:HG3	1.97	0.47
1:A:112:GLU:OE1	1:A:234:PRO:HA	2.15	0.47
1:B:271:VAL:O	1:B:272:VAL:C	2.59	0.46
1:A:147:ARG:NH1	1:B:171:GLU:OE2	2.48	0.46
1:B:262:ILE:O	1:B:265:ASP:HB2	2.16	0.46
1:C:47:VAL:HG13	1:C:48:PRO:HD3	1.98	0.46
1:A:47:VAL:HG22	1:A:48:PRO:HD3	1.99	0.45
1:A:167:MET:HE2	1:B:147:ARG:HD3	1.97	0.45
1:C:165:HIS:CE1	1:C:266:GLU:OE1	2.70	0.45
1:A:150:GLY:HA3	1:A:292:VAL:HG11	1.98	0.45
1:A:47:VAL:HG21	1:B:284:LEU:HD23	1.98	0.45
1:D:59:SER:OG	1:D:160:GLU:OE1	2.28	0.45
1:A:147:ARG:HD3	1:B:167:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LEU:O	1:D:47:VAL:HG13	2.17	0.45
1:A:171:GLU:OE1	1:A:240:PRO:HB3	2.16	0.45
1:A:167:MET:CE	1:B:147:ARG:HA	2.47	0.45
1:D:73:VAL:HB	1:D:263:ARG:HH11	1.80	0.45
1:B:54:VAL:CG2	1:B:242:VAL:HG13	2.47	0.45
1:B:133:GLY:O	1:B:134:GLY:C	2.60	0.45
1:B:209:VAL:O	1:B:210:GLY:C	2.58	0.45
1:D:175:PRO:CB	1:D:179:LEU:HD12	2.47	0.45
1:D:216:ALA:O	1:D:217:VAL:C	2.60	0.45
1:B:220:TYR:HB3	1:B:263:ARG:HB2	1.99	0.44
1:B:221:THR:HG22	1:B:263:ARG:HE	1.81	0.44
1:D:252:ASN:O	1:D:253:ALA:C	2.60	0.44
1:A:87:LEU:O	1:A:91:SER:OG	2.32	0.44
1:C:122:LEU:HD13	5:C:505:9AU:CAX	2.47	0.44
1:B:175:PRO:CB	1:B:179:LEU:HD12	2.48	0.44
1:B:241:GLU:O	1:B:242:VAL:C	2.61	0.44
1:A:32:VAL:O	1:A:32:VAL:HG13	2.17	0.43
1:A:167:MET:HE2	1:B:147:ARG:HA	2.00	0.43
1:A:207:ARG:HD3	1:A:274:HIS:HD2	1.83	0.43
1:A:289:ASN:O	1:A:292:VAL:HG22	2.18	0.43
1:B:45:GLU:H	1:B:45:GLU:CD	2.25	0.43
1:B:163:ARG:O	1:B:167:MET:HG2	2.17	0.43
1:B:185:ILE:C	1:B:185:ILE:HD12	2.43	0.43
1:B:187:GLN:O	1:B:188:ALA:C	2.60	0.43
1:A:41:LEU:HD22	1:B:78:LYS:HA	2.00	0.43
1:B:54:VAL:HG22	1:B:242:VAL:HG13	2.01	0.43
1:C:267:ALA:O	1:C:270:ARG:HB3	2.17	0.43
1:D:152:ILE:HG22	1:D:156:LEU:HD22	2.01	0.43
1:A:268:GLU:O	1:A:272:VAL:HG23	2.19	0.43
1:B:79:LYS:HE3	1:C:256:ARG:HD3	1.99	0.43
1:B:289:ASN:O	1:B:290:PRO:C	2.61	0.43
1:D:272:VAL:HA	1:D:291:PHE:CZ	2.54	0.43
1:B:282:LYS:O	1:B:283:ARG:HB2	2.18	0.42
1:C:283:ARG:HA	1:C:285:GLN:HE21	1.84	0.42
1:A:187:GLN:NE2	1:B:139:LEU:HB3	2.34	0.42
1:C:67:LEU:HB2	1:C:68:PRO:HD3	2.01	0.42
1:C:185:ILE:CD1	1:C:189:ILE:CD1	2.97	0.42
1:B:89:TYR:OH	1:C:225:ARG:NE	2.43	0.42
1:C:89:TYR:CE1	1:C:93:ARG:HD3	2.54	0.42
1:D:71:GLU:OE2	1:D:256:ARG:NH2	2.47	0.42
1:D:211:TYR:O	1:D:215:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:THR:HG23	5:C:505:9AU:CAA	2.50	0.42
1:C:205:VAL:O	1:C:209:VAL:HG23	2.20	0.42
1:A:92:VAL:HG23	1:A:208:PHE:CD1	2.54	0.42
1:B:65:TRP:CB	1:B:70:ILE:HD13	2.49	0.42
1:D:96:ARG:NH1	1:D:215:GLU:OE1	2.49	0.42
1:D:144:TYR:O	1:D:146:THR:HG23	2.20	0.42
1:A:96:ARG:CA	5:A:505:9AU:CAD	2.95	0.42
1:A:153:ASN:O	1:A:157:VAL:HG13	2.19	0.42
1:B:177:LEU:N	1:B:178:PRO:CD	2.83	0.42
1:B:34:GLY:O	1:B:38:LEU:HG	2.20	0.42
1:B:86:THR:O	1:B:87:LEU:C	2.62	0.42
1:D:54:VAL:HG13	1:D:242:VAL:HA	2.02	0.42
1:D:153:ASN:O	1:D:154:THR:C	2.63	0.42
1:A:93:ARG:NE	1:D:229:GLU:OE2	2.47	0.41
5:B:505:9AU:OAF	5:B:505:9AU:CAI	2.68	0.41
1:C:122:LEU:HD13	5:C:505:9AU:CAW	2.50	0.41
1:D:144:TYR:O	1:D:145:MET:C	2.63	0.41
1:C:125:VAL:O	1:C:129:PRO:HD3	2.20	0.41
1:D:47:VAL:N	1:D:48:PRO:CD	2.82	0.41
1:A:122:LEU:HD13	5:A:505:9AU:CAW	2.50	0.41
1:A:145:MET:HG3	1:B:166:LEU:HD21	2.02	0.41
1:D:119:CYS:O	1:D:123:GLU:HG2	2.20	0.41
1:A:204:PHE:CD2	1:A:204:PHE:C	2.98	0.41
1:A:267:ALA:O	1:A:271:VAL:HG22	2.20	0.41
1:C:198:TYR:CE1	1:C:202:PRO:HB3	2.55	0.41
1:B:132:VAL:O	1:B:136:LEU:HD22	2.20	0.41
1:D:175:PRO:HB2	1:D:179:LEU:HD12	2.03	0.41
1:A:241:GLU:O	1:A:242:VAL:C	2.61	0.41
1:B:128:VAL:N	1:B:129:PRO:CD	2.84	0.41
1:B:263:ARG:HD3	6:B:611:HOH:O	2.21	0.41
1:B:85:ASP:CG	1:B:207:ARG:HE	2.29	0.41
1:B:144:TYR:O	1:B:145:MET:C	2.64	0.41
1:B:162:GLU:O	1:B:165:HIS:HB2	2.21	0.41
1:C:110:ILE:CG2	1:C:232:LEU:HD13	2.50	0.41
1:B:58:SER:HB3	1:B:164:MET:HE2	2.03	0.40
1:C:54:VAL:HG22	1:C:242:VAL:HA	2.03	0.40
1:C:80:PRO:CB	1:C:85:ASP:HB3	2.51	0.40
1:A:93:ARG:HA	1:A:93:ARG:HD2	1.94	0.40
1:C:221:THR:O	1:C:222:GLY:C	2.64	0.40
1:D:172:LEU:HD22	1:D:236:LYS:HB3	2.03	0.40
1:D:54:VAL:HG11	1:D:245:VAL:HG13	2.03	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%)	240 (92%)	17 (6%)	5 (2%)	6	15
1	B	261/329 (79%)	230 (88%)	30 (12%)	1 (0%)	30	52
1	C	264/329 (80%)	247 (94%)	14 (5%)	3 (1%)	11	27
1	D	263/329 (80%)	235 (89%)	22 (8%)	6 (2%)	5	12
All	All	1050/1316 (80%)	952 (91%)	83 (8%)	15 (1%)	9	22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	294	LEU
1	D	54	VAL
1	C	44	LEU
1	A	281	GLU
1	C	234	PRO
1	D	59	SER
1	D	61	ASP
1	D	253	ALA
1	A	152	ILE
1	B	126	ALA
1	C	195	LEU
1	D	210	GLY
1	D	234	PRO
1	A	242	VAL

5.3.2 Protein sidechains ⓘ

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%)	211 (88%)	28 (12%)	5	12
1	B	238/292 (82%)	210 (88%)	28 (12%)	5	12
1	C	241/292 (82%)	213 (88%)	28 (12%)	5	13
1	D	240/292 (82%)	211 (88%)	29 (12%)	5	12
All	All	958/1168 (82%)	845 (88%)	113 (12%)	5	12

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

Mol	Chain	Res	Type
1	A	40	ARG
1	A	44	LEU
1	A	47	VAL
1	A	50	VAL
1	A	54	VAL
1	A	66	SER
1	A	86	THR
1	A	98	LEU
1	A	101	THR
1	A	106	ARG
1	A	132	VAL
1	A	136	LEU
1	A	145	MET
1	A	156	LEU
1	A	157	VAL
1	A	166	LEU
1	A	170	ILE
1	A	179	LEU
1	A	182	SER
1	A	196	VAL
1	A	233	ARG
1	A	242	VAL
1	A	245	VAL
1	A	258	LEU

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Mol	Chain	Res	Type
1	A	271	VAL
1	A	275	THR
1	A	284	LEU
1	A	288	VAL
1	B	40	ARG
1	B	44	LEU
1	B	45	GLU
1	B	47	VAL
1	B	50	VAL
1	B	52	LEU
1	B	60	GLU
1	B	81	ASN
1	B	87	LEU
1	B	106	ARG
1	B	120	LEU
1	B	132	VAL
1	B	136	LEU
1	B	156	LEU
1	B	166	LEU
1	B	170	ILE
1	B	179	LEU
1	B	185	ILE
1	B	196	VAL
1	B	221	THR
1	B	225	ARG
1	B	233	ARG
1	B	242	VAL
1	B	260	ASN
1	B	271	VAL
1	B	284	LEU
1	B	285	GLN
1	B	288	VAL
1	C	44	LEU
1	C	47	VAL
1	C	50	VAL
1	C	52	LEU
1	C	54	VAL
1	C	90	ARG
1	C	106	ARG
1	C	110	ILE
1	C	132	VAL
1	C	136	LEU

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Mol	Chain	Res	Type
1	C	156	LEU
1	C	166	LEU
1	C	179	LEU
1	C	185	ILE
1	C	186	THR
1	C	192	LEU
1	C	196	VAL
1	C	231	ARG
1	C	233	ARG
1	C	242	VAL
1	C	245	VAL
1	C	263	ARG
1	C	271	VAL
1	C	274	HIS
1	C	281	GLU
1	C	284	LEU
1	C	285	GLN
1	C	288	VAL
1	D	44	LEU
1	D	45	GLU
1	D	47	VAL
1	D	54	VAL
1	D	61	ASP
1	D	81	ASN
1	D	87	LEU
1	D	98	LEU
1	D	106	ARG
1	D	110	ILE
1	D	118	ARG
1	D	132	VAL
1	D	136	LEU
1	D	154	THR
1	D	156	LEU
1	D	157	VAL
1	D	166	LEU
1	D	170	ILE
1	D	179	LEU
1	D	221	THR
1	D	225	ARG
1	D	233	ARG
1	D	242	VAL
1	D	245	VAL

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Mol	Chain	Res	Type
1	D	271	VAL
1	D	284	LEU
1	D	285	GLN
1	D	287	SER
1	D	294	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	HIS
1	A	187	GLN
1	A	237	ASN
1	A	269	HIS
1	A	273	ASN
1	B	153	ASN
1	B	161	ASN
1	B	187	GLN
1	B	269	HIS
1	B	274	HIS
1	B	280	HIS
1	C	72	ASN
1	C	248	ASN
1	C	269	HIS
1	C	273	ASN
1	C	274	HIS
1	C	285	GLN
1	C	286	ASN
1	D	248	ASN
1	D	260	ASN
1	D	269	HIS
1	D	273	ASN
1	D	274	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - leaving 8 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
5	9AU	A	505	-	28,28,28	1.37	3 (10%)	36,37,37	1.84	7 (19%)
4	OXY	B	504	-	1,1,1	0.10	0	-		
5	9AU	D	505	-	28,28,28	1.19	2 (7%)	36,37,37	1.67	9 (25%)
4	OXY	C	504	2	1,1,1	0.13	0	-		
5	9AU	B	505	-	28,28,28	1.36	2 (7%)	36,37,37	2.24	7 (19%)
4	OXY	A	504	-	1,1,1	0.08	0	-		
4	OXY	D	504	-	1,1,1	0.12	0	-		
5	9AU	C	505	-	28,28,28	1.23	2 (7%)	36,37,37	1.79	7 (19%)

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
5	9AU	A	505	-	-	4/17/17/17	0/2/2/2
5	9AU	D	505	-	-	5/17/17/17	0/2/2/2
5	9AU	B	505	-	-	4/17/17/17	0/2/2/2
5	9AU	C	505	-	-	3/17/17/17	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	9AU	CAP-CAI	-4.22	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	505	9AU	CBA-CAW	-3.91	1.39	1.45
5	A	505	9AU	CAP-CAI	-3.75	1.44	1.50
5	A	505	9AU	CBA-CAW	-3.73	1.39	1.45
5	C	505	9AU	CBA-CAW	-3.51	1.40	1.45
5	C	505	9AU	CAP-CAI	-3.39	1.45	1.50
5	B	505	9AU	CBA-CAW	-2.64	1.41	1.45
5	D	505	9AU	CAP-CAI	-2.45	1.46	1.50
5	A	505	9AU	CAP-CAX	-2.09	1.47	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	9AU	CAP-CAI-CAV	-9.60	110.29	126.83
5	C	505	9AU	CAP-CAI-CAV	-6.11	116.31	126.83
5	A	505	9AU	CAP-CAI-CAV	-6.05	116.42	126.83
5	B	505	9AU	CBA-CAW-CAX	-4.40	118.36	120.99
5	D	505	9AU	OAS-CAZ-CAL	3.76	121.26	116.25
5	A	505	9AU	CBA-CAW-CAX	-3.49	118.90	120.99
5	B	505	9AU	OAF-CAW-CBA	3.37	122.37	115.69
5	D	505	9AU	CAI-CAP-CAX	3.29	120.18	112.08
5	B	505	9AU	CAI-CAP-CAX	3.09	119.69	112.08
5	D	505	9AU	CAP-CAI-CAV	-3.02	121.63	126.83
5	C	505	9AU	CAZ-CBA-CAW	2.99	120.48	117.81
5	A	505	9AU	CAO-CAR-CAV	-2.92	103.52	113.19
5	C	505	9AU	OAS-CAY-CAX	2.77	121.31	117.86
5	C	505	9AU	OAS-CAZ-CAL	2.73	119.89	116.25
5	A	505	9AU	CAZ-CBA-CAW	2.72	120.24	117.81
5	C	505	9AU	OAS-CAZ-CBA	-2.66	119.15	121.57
5	D	505	9AU	OAS-CAY-OAE	2.57	119.61	116.22
5	D	505	9AU	CAD-CAV-CAR	2.47	119.52	115.23
5	D	505	9AU	OAE-CAY-CAX	-2.44	119.84	125.55
5	A	505	9AU	OAS-CAY-CAX	2.41	120.86	117.86
5	C	505	9AU	CAI-CAP-CAX	2.37	117.93	112.08
5	B	505	9AU	CAZ-CBA-CAW	2.37	119.93	117.81
5	B	505	9AU	CAO-CAR-CAV	-2.37	105.34	113.19
5	B	505	9AU	OAS-CAY-CAX	2.25	120.65	117.86
5	D	505	9AU	CAP-CAX-CAY	2.22	119.61	116.36
5	A	505	9AU	OAS-CAZ-CAL	2.21	119.20	116.25
5	D	505	9AU	OAS-CAY-CAX	2.16	120.54	117.86
5	D	505	9AU	CAZ-CBA-CAW	2.05	119.64	117.81
5	A	505	9AU	OAF-CAW-CBA	2.02	119.69	115.69
5	C	505	9AU	OAE-CAY-CAX	-2.01	120.84	125.55

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	9AU	CAI-CAP-CAX-CAY
5	A	505	9AU	CAI-CAP-CAX-CAW
5	B	505	9AU	CAI-CAP-CAX-CAY
5	B	505	9AU	CAI-CAP-CAX-CAW
5	C	505	9AU	CAI-CAP-CAX-CAY
5	C	505	9AU	CAI-CAP-CAX-CAW
5	D	505	9AU	CAI-CAP-CAX-CAY
5	D	505	9AU	CAI-CAP-CAX-CAW
5	B	505	9AU	CAH-CAO-CAR-CAV
5	B	505	9AU	CAG-CAN-CAQ-CAU
5	A	505	9AU	CAH-CAO-CAR-CAV
5	C	505	9AU	CAH-CAO-CAR-CAV
5	D	505	9AU	CAH-CAO-CAR-CAV
5	A	505	9AU	CAG-CAN-CAQ-CAU
5	D	505	9AU	CAO-CAR-CAV-CAD
5	D	505	9AU	CAO-CAR-CAV-CAI

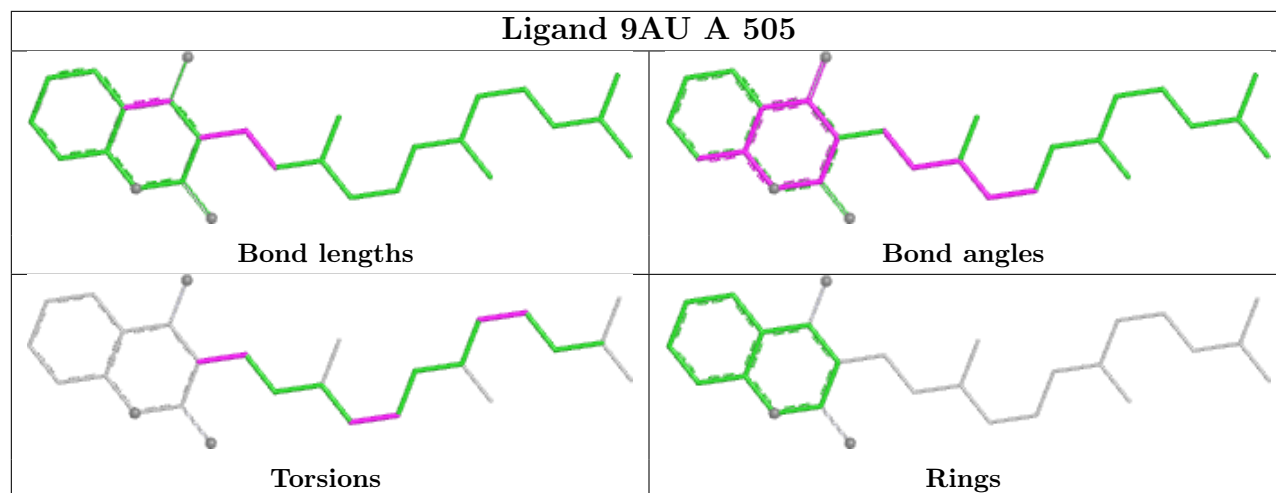
There are no ring outliers.

4 monomers are involved in 14 short contacts:

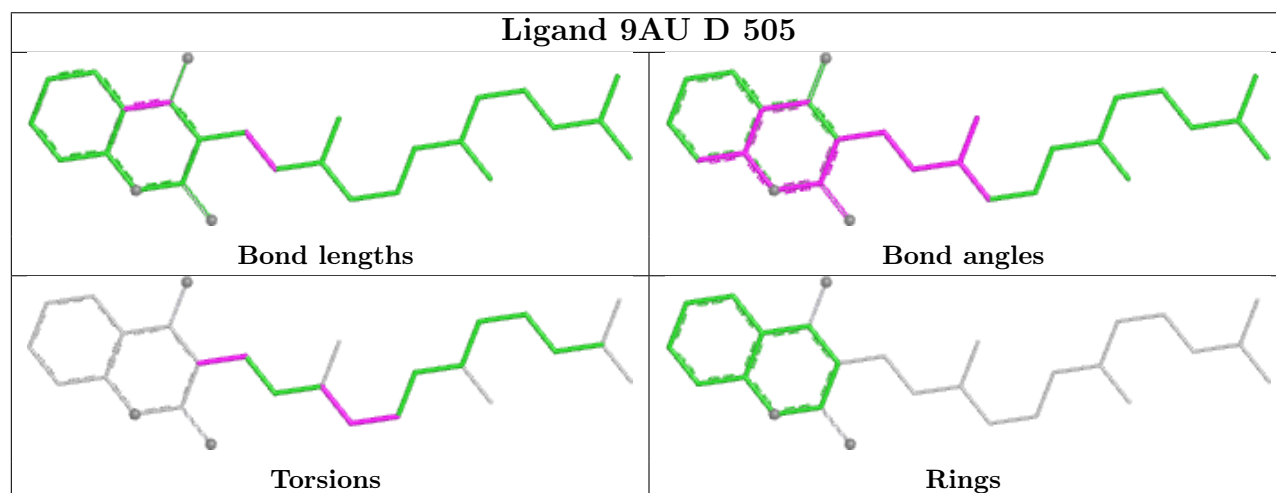
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	9AU	4	0
5	D	505	9AU	2	0
5	B	505	9AU	2	0
5	C	505	9AU	6	0

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 than 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.

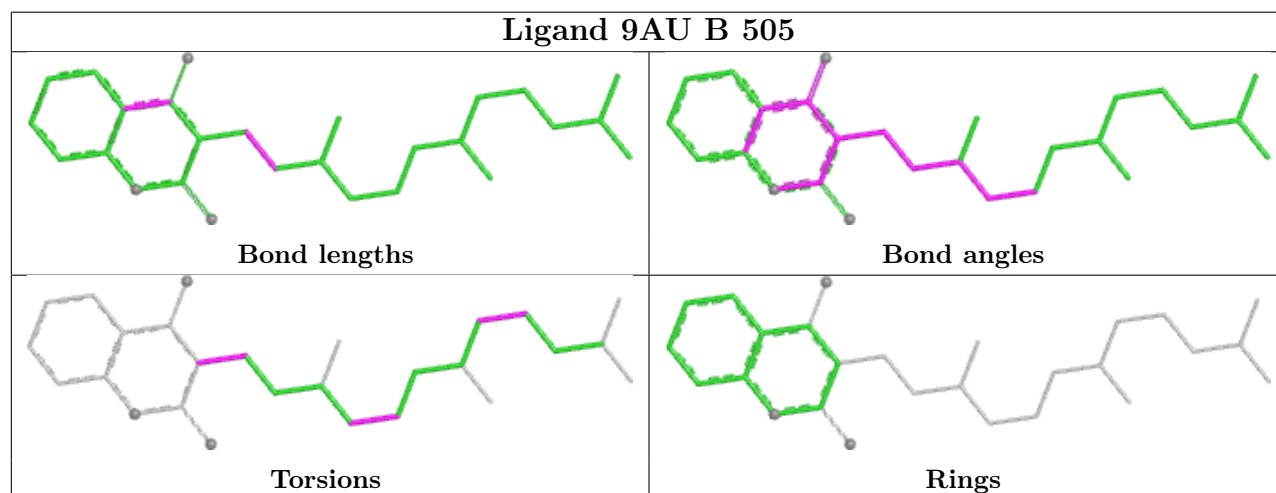
Ligand 9AU A 505

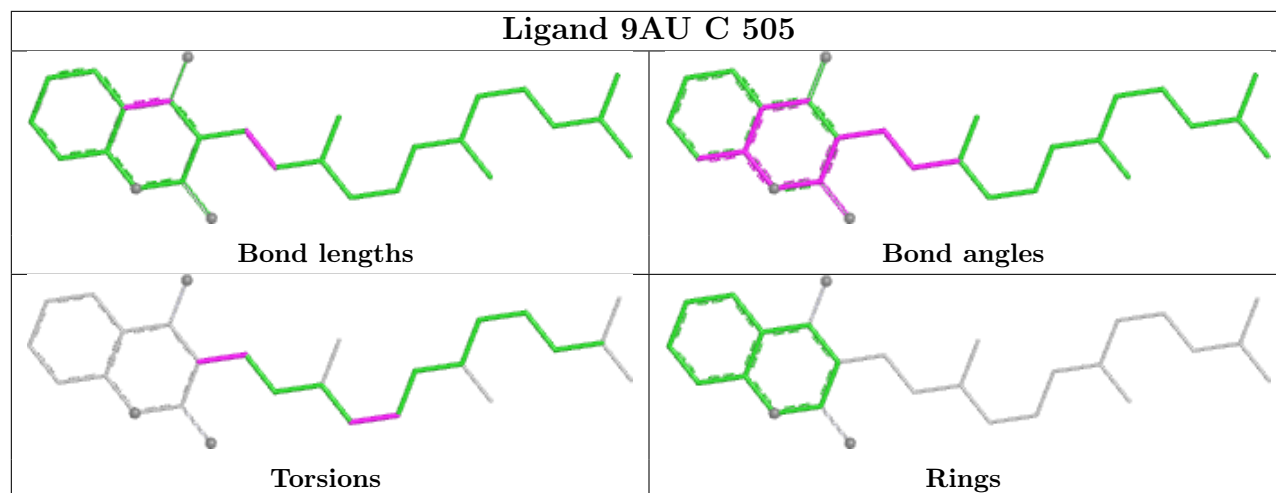


Ligand 9AU D 505



Ligand 9AU B 505





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, 95th 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%)	0.41	13 (4%) 35 32	23, 39, 58, 91	0
1	B	263/329 (79%)	0.47	18 (6%) 23 21	19, 38, 60, 94	0
1	C	266/329 (80%)	0.80	31 (11%) 9 8	27, 46, 97, 163	0
1	D	265/329 (80%)	1.03	38 (14%) 6 5	34, 55, 118, 159	0
All	All	1058/1316 (80%)	0.68	100 (9%) 14 12	19, 44, 84, 163	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	110	ILE	8.5
1	B	294	LEU	7.2
1	C	104	LEU	7.1
1	C	105	TYR	6.7
1	D	104	LEU	6.7
1	C	107	PHE	6.4
1	C	110	ILE	6.0
1	D	235	THR	6.0
1	D	105	TYR	5.9
1	D	107	PHE	5.9
1	D	233	ARG	5.5
1	D	236	LYS	5.4
1	D	108	GLY	5.3
1	D	109	SER	5.0
1	D	234	PRO	4.9
1	D	102	PHE	4.9
1	C	102	PHE	4.6
1	A	107	PHE	4.5
1	B	293	VAL	4.5
1	D	232	LEU	4.5
1	C	101	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	101	THR	4.2
1	D	231	ARG	4.2
1	C	106	ARG	4.1
1	D	106	ARG	4.1
1	C	221	THR	4.0
1	D	237	ASN	3.8
1	C	236	LYS	3.8
1	C	237	ASN	3.8
1	D	238	ASP	3.7
1	C	235	THR	3.6
1	C	121	PHE	3.6
1	D	97	TRP	3.5
1	B	234	PRO	3.4
1	B	238	ASP	3.4
1	A	32	VAL	3.4
1	C	32	VAL	3.4
1	D	32	VAL	3.4
1	B	32	VAL	3.4
1	C	238	ASP	3.3
1	A	294	LEU	3.2
1	D	111	THR	3.2
1	B	226	ALA	3.2
1	B	106	ARG	3.1
1	A	45	GLU	3.0
1	D	174	GLN	3.0
1	C	114	LYS	3.0
1	A	295	LYS	2.9
1	B	230	GLY	2.8
1	B	83	LEU	2.8
1	B	107	PHE	2.8
1	C	111	THR	2.8
1	C	109	SER	2.8
1	D	79	LYS	2.7
1	A	234	PRO	2.7
1	D	98	LEU	2.6
1	C	112	GLU	2.6
1	D	196	VAL	2.6
1	C	115	VAL	2.6
1	C	244	ARG	2.5
1	D	283	ARG	2.5
1	B	113	SER	2.5
1	C	79	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	234	PRO	2.5
1	B	221	THR	2.5
1	D	87	LEU	2.5
1	B	93	ARG	2.4
1	D	239	VAL	2.4
1	A	227	ILE	2.4
1	A	106	ARG	2.4
1	B	46	THR	2.4
1	D	40	ARG	2.3
1	C	232	LEU	2.3
1	C	296	LYS	2.3
1	C	116	ILE	2.3
1	D	170	ILE	2.3
1	D	216	ALA	2.3
1	B	225	ARG	2.3
1	D	83	LEU	2.3
1	C	189	ILE	2.2
1	B	104	LEU	2.2
1	A	126	ALA	2.2
1	A	238	ASP	2.2
1	C	177	LEU	2.2
1	D	132	VAL	2.2
1	C	204	PHE	2.2
1	D	191	TYR	2.2
1	C	226	ALA	2.2
1	A	233	ARG	2.1
1	C	98	LEU	2.1
1	D	103	SER	2.1
1	D	81	ASN	2.1
1	D	185	ILE	2.1
1	D	181	VAL	2.1
1	B	54	VAL	2.0
1	A	74	ALA	2.0
1	D	253	ALA	2.0
1	A	64	THR	2.0
1	B	101	THR	2.0
1	C	97	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

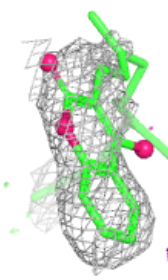
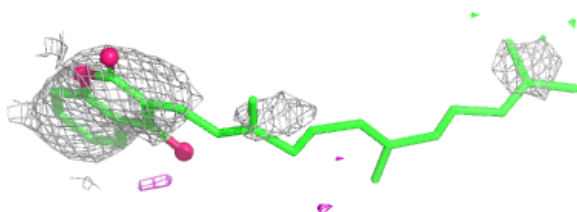
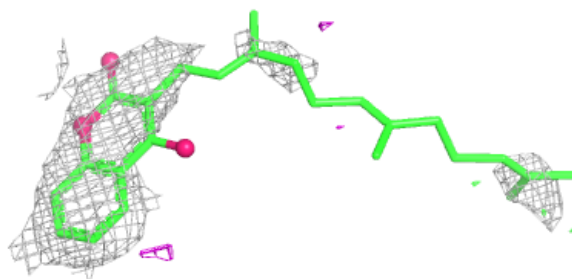
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	9AU	D	505	27/27	0.82	0.35	77,108,124,126	0
5	9AU	C	505	27/27	0.84	0.22	56,64,69,73	0
5	9AU	A	505	27/27	0.88	0.18	51,62,68,73	0
5	9AU	B	505	27/27	0.89	0.18	37,49,79,82	0
4	OXY	A	504	2/2	0.92	0.21	29,29,29,30	0
4	OXY	D	504	2/2	0.94	0.08	45,45,45,48	0
4	OXY	B	504	2/2	0.95	0.22	43,43,43,48	0
4	OXY	C	504	2/2	0.97	0.09	48,48,48,50	0
3	OH	A	503	1/1	0.97	0.12	16,16,16,16	0
2	FE	A	501	1/1	0.99	0.02	44,44,44,44	0
3	OH	C	503	1/1	0.99	0.04	24,24,24,24	0
2	FE	A	502	1/1	0.99	0.03	38,38,38,38	0
2	FE	C	501	1/1	0.99	0.04	49,49,49,49	0
2	FE	D	501	1/1	0.99	0.03	51,51,51,51	0
2	FE	B	501	1/1	1.00	0.02	28,28,28,28	0
3	OH	B	503	1/1	1.00	0.04	40,40,40,40	0
2	FE	C	502	1/1	1.00	0.03	35,35,35,35	0
3	OH	D	503	1/1	1.00	0.05	14,14,14,14	0
2	FE	B	502	1/1	1.00	0.02	27,27,27,27	0
2	FE	D	502	1/1	1.00	0.02	56,56,56,56	0

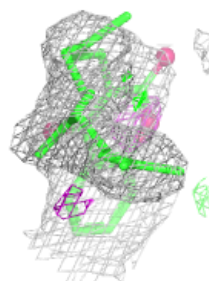
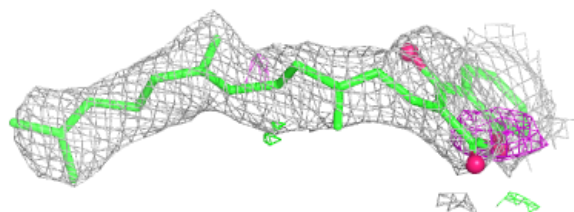
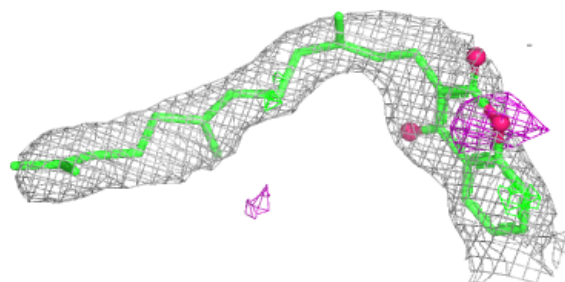
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9AU D 505:

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

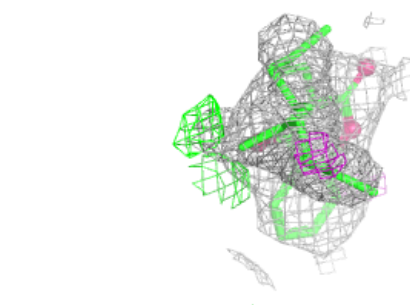
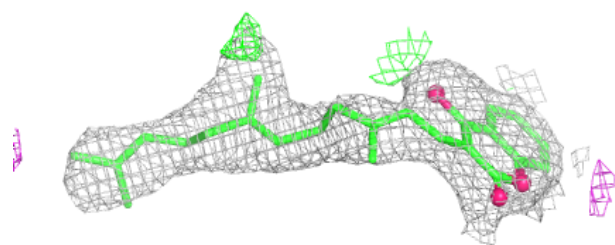
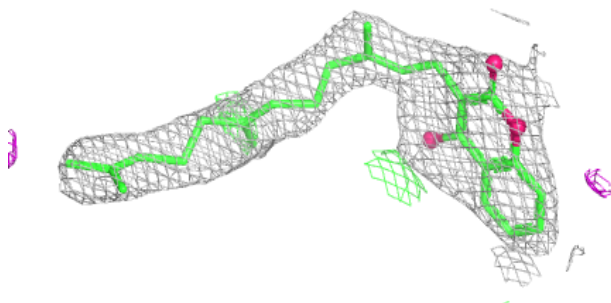
**Electron density around 9AU C 505:**

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

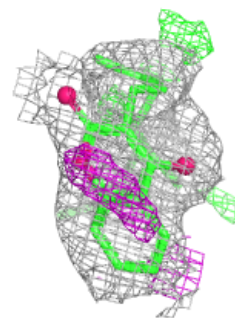
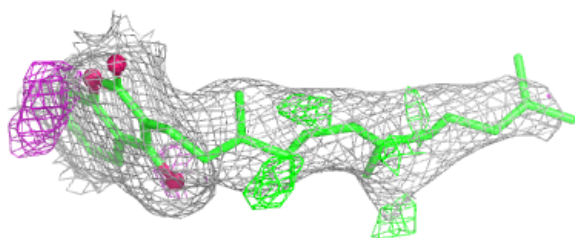
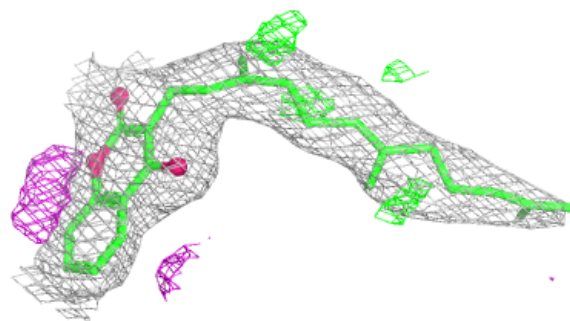


Electron density around 9AU A 505:

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

**Electron density around 9AU B 505:**

$2mF_o-DF_c$ (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.