



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1HXC / pdb_00001hxc
Title : CRYSTAL STRUCTURE OF TEAS C440W
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Deposited on : 2001-01-12
Resolution : 2.25 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	:	4-5-2 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

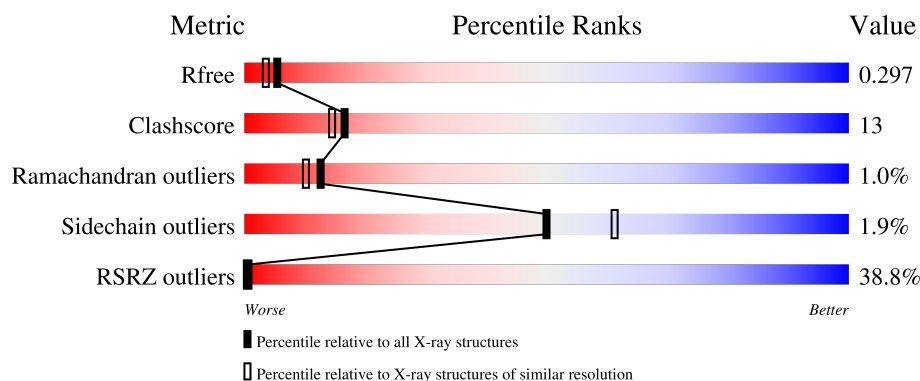
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	548	36% 70% 21% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FHP	A	900	-	-	X	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4263 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.

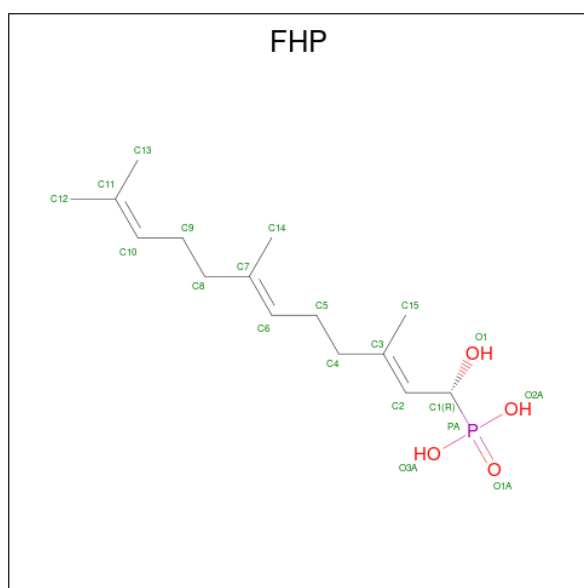
- Molecule 1 is a protein called 5-EPI-ARISTOLOCHENE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	4192	2682	691	801	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	TRP	CYS	engineered mutation	UNP Q40577
A	532	GLU	LYS	see remark 999	UNP Q40577

- Molecule 2 is 1-HYDROXY-3,7,11-TRIMETHYLDODECA-2,6,10-TRIENE PHOSPHONIC ACID (CCD ID: FHP) (formula: $C_{15}H_{27}O_4P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	20	15	4	1	0	0

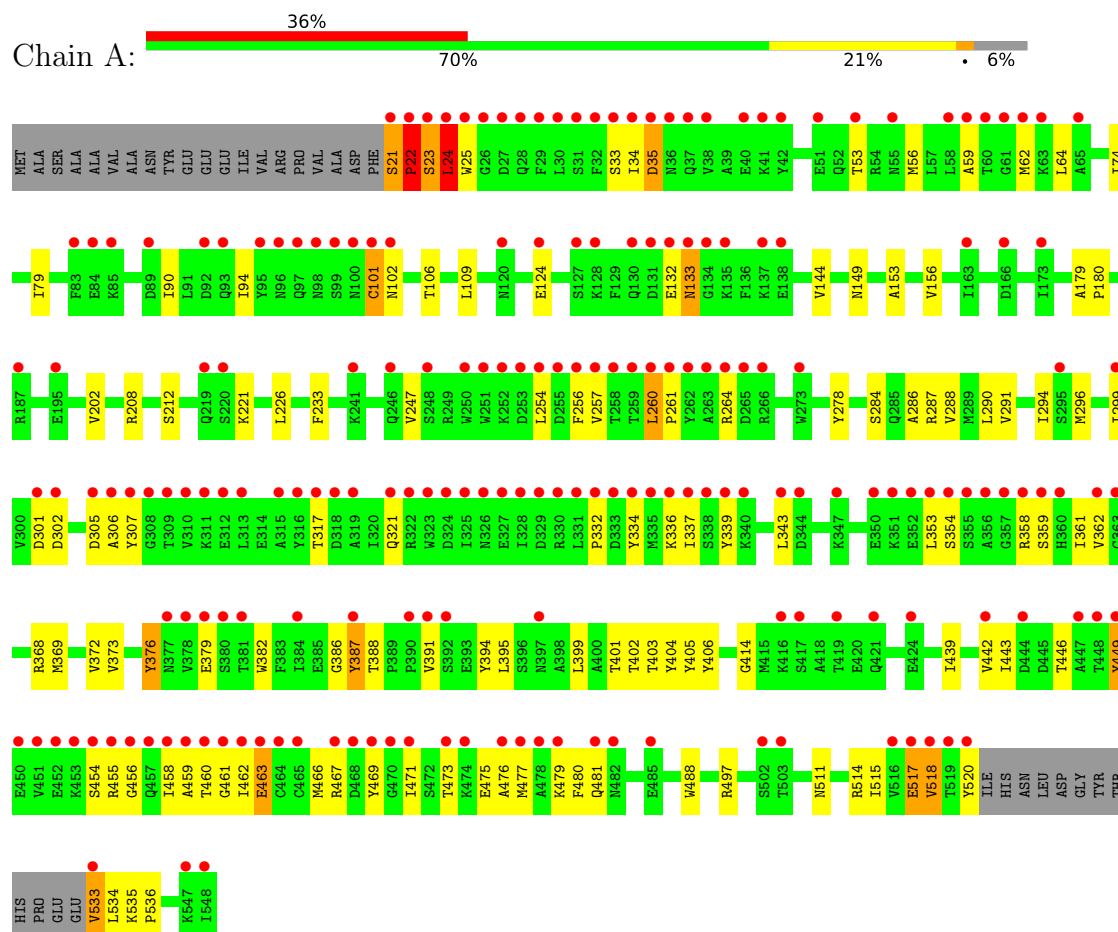
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		

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: 5-EPI-ARISTOLOCHENE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.12Å 126.12Å 120.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 50.00 – 2.27	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-2.25) 94.7 (50.00-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 2.27Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.296 0.278 , 0.297	Depositor DCC
R_{free} test set	1996 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4263	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: FHP

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	0.63	7/4281 (0.2%)	1.01	23/5803 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	LEU	C-O	13.54	1.41	1.24
1	A	518	VAL	N-CA	-11.56	1.32	1.46
1	A	517	GLU	CA-C	-9.95	1.39	1.52
1	A	517	GLU	C-N	-7.39	1.24	1.33
1	A	21	SER	C-O	-6.13	1.11	1.23
1	A	518	VAL	C-O	-5.34	1.17	1.24
1	A	23	SER	CA-C	-5.01	1.46	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	GLU	CA-C-O	15.27	137.80	119.79
1	A	24	LEU	O-C-N	10.31	136.31	122.59
1	A	517	GLU	CA-C-N	-10.13	104.34	120.55
1	A	517	GLU	C-N-CA	-10.13	104.34	120.55
1	A	260	LEU	CA-C-N	8.46	128.11	119.82
1	A	260	LEU	C-N-CA	8.46	128.11	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	ARG	N-CA-C	-8.16	103.79	112.93
1	A	261	PRO	N-CA-C	7.18	123.24	113.98
1	A	23	SER	O-C-N	6.70	131.05	123.27
1	A	402	THR	N-CA-C	-6.65	104.65	112.89
1	A	520	TYR	CA-CB-CG	-6.28	102.59	113.90
1	A	102	ASN	N-CA-C	6.17	123.93	110.80
1	A	24	LEU	CA-C-O	-6.00	111.94	120.51
1	A	404	TYR	N-CA-C	5.97	117.79	111.28
1	A	212	SER	N-CA-C	5.81	118.83	111.69
1	A	144	VAL	N-CA-C	5.77	115.96	110.42
1	A	405	TYR	N-CA-C	-5.74	105.16	111.82
1	A	306	ALA	N-CA-C	5.50	120.28	111.81
1	A	257	VAL	N-CA-C	-5.35	105.06	112.50
1	A	533	VAL	CB-CA-C	-5.33	101.28	111.40
1	A	463	GLU	N-CA-C	-5.33	105.55	111.36
1	A	387	TYR	N-CA-C	5.28	117.33	109.25
1	A	101	CYS	N-CA-C	-5.13	98.68	108.17

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	PRO	Mainchain
1	A	376	TYR	Sidechain
1	A	449	TYR	Sidechain

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	4192	0	4145	103	0
2	A	20	0	25	17	0
3	A	51	0	0	0	0
All	All	4263	0	4170	108	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 13.

All (108) 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:401:THR:O	2:A:900:FHP:H152	1.48	1.13
1:A:24:LEU:H	1:A:24:LEU:HD23	1.04	1.08
2:A:900:FHP:H133	2:A:900:FHP:H82	1.33	1.07
1:A:301:ASP:CG	2:A:900:FHP:H2	1.80	1.05
1:A:386:GLY:HA2	1:A:458:ILE:HD13	1.32	1.05
1:A:301:ASP:OD1	2:A:900:FHP:H2	1.56	1.02
1:A:202:VAL:HG23	1:A:518:VAL:HG21	1.44	0.98
1:A:386:GLY:CA	1:A:458:ILE:HD13	1.96	0.96
1:A:401:THR:O	2:A:900:FHP:C15	2.16	0.93
1:A:458:ILE:HG13	1:A:459:ALA:N	1.84	0.92
2:A:900:FHP:H82	2:A:900:FHP:C13	2.03	0.89
1:A:24:LEU:HD23	1:A:24:LEU:N	1.89	0.87
1:A:23:SER:C	1:A:25:TRP:H	1.77	0.87
1:A:301:ASP:OD1	2:A:900:FHP:C2	2.22	0.86
1:A:386:GLY:C	1:A:458:ILE:CD1	2.51	0.83
1:A:287:ARG:O	1:A:291:VAL:HG23	1.81	0.79
1:A:376:TYR:CE2	2:A:900:FHP:C1	2.66	0.79
1:A:387:TYR:N	1:A:458:ILE:CD1	2.47	0.77
1:A:376:TYR:CE2	2:A:900:FHP:O1	2.38	0.77
1:A:379:GLU:OE2	2:A:900:FHP:O2A	2.02	0.76
1:A:23:SER:C	1:A:25:TRP:N	2.39	0.76
1:A:376:TYR:CE2	2:A:900:FHP:H1	2.20	0.75
1:A:359:SER:O	1:A:362:VAL:HG23	1.89	0.73
1:A:488:TRP:HZ2	1:A:517:GLU:OE2	1.73	0.71
1:A:260:LEU:HD11	1:A:337:ILE:HB	1.71	0.71
2:A:900:FHP:C13	2:A:900:FHP:C8	2.69	0.71
1:A:301:ASP:OD1	2:A:900:FHP:O1	2.08	0.70
1:A:358:ARG:O	1:A:361:ILE:HG12	1.92	0.70
1:A:514:ARG:O	1:A:517:GLU:OE1	2.09	0.70
1:A:471:ILE:HB	1:A:475:GLU:HB2	1.73	0.69
1:A:376:TYR:HE2	2:A:900:FHP:H1	1.56	0.69
1:A:514:ARG:HA	1:A:517:GLU:OE1	1.91	0.69
1:A:109:LEU:HB2	1:A:149:ASN:HD22	1.56	0.68
1:A:535:LYS:HB3	1:A:536:PRO:HD3	1.75	0.68
1:A:462:ILE:HD13	1:A:477:MET:HG2	1.76	0.68
1:A:353:LEU:HB2	1:A:359:SER:HA	1.75	0.67
1:A:24:LEU:H	1:A:24:LEU:CD2	1.82	0.67
1:A:533:VAL:HG22	1:A:533:VAL:O	1.96	0.66
1:A:386:GLY:CA	1:A:458:ILE:CD1	2.73	0.66
1:A:442:VAL:HG13	1:A:480:PHE:HB3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HB2	1:A:149:ASN:ND2	2.12	0.64
1:A:382:TRP:O	1:A:458:ILE:HD11	1.97	0.64
1:A:386:GLY:C	1:A:458:ILE:HD12	2.21	0.64
1:A:317:THR:O	1:A:321:GLN:HG2	1.97	0.63
1:A:64:LEU:HD23	1:A:101:CYS:HB2	1.79	0.63
1:A:74:ILE:HG23	1:A:79:ILE:HG13	1.80	0.62
1:A:101:CYS:SG	1:A:106:THR:HG21	2.42	0.59
1:A:488:TRP:CZ2	1:A:517:GLU:OE2	2.56	0.59
1:A:153:ALA:O	1:A:156:VAL:HG22	2.03	0.59
1:A:462:ILE:O	1:A:466:MET:HG3	2.02	0.58
1:A:442:VAL:HG11	1:A:480:PHE:O	2.03	0.58
1:A:458:ILE:HG13	1:A:459:ALA:H	1.67	0.58
1:A:386:GLY:C	1:A:458:ILE:HD13	2.22	0.57
1:A:301:ASP:OD1	2:A:900:FHP:C1	2.52	0.57
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.87	0.56
1:A:387:TYR:N	1:A:458:ILE:HD11	2.20	0.56
1:A:388:THR:HG21	1:A:467:ARG:HD2	1.88	0.56
1:A:90:ILE:O	1:A:94:ILE:HG13	2.06	0.55
1:A:254:LEU:HD13	1:A:256:PHE:CE1	2.42	0.55
1:A:511:ASN:O	1:A:515:ILE:HG13	2.07	0.55
1:A:454:SER:C	1:A:456:GLY:H	2.13	0.54
1:A:449:TYR:CG	1:A:449:TYR:O	2.61	0.54
1:A:439:ILE:O	1:A:443:ILE:HG12	2.07	0.54
1:A:458:ILE:CG1	1:A:459:ALA:N	2.67	0.54
1:A:533:VAL:HG13	1:A:534:LEU:HG	1.89	0.53
1:A:59:ALA:HB3	1:A:62:MET:SD	2.49	0.53
1:A:387:TYR:N	1:A:458:ILE:HD12	2.23	0.53
1:A:296:MET:HE3	1:A:299:ILE:HD12	1.91	0.52
1:A:286:ALA:HA	1:A:414:GLY:HA3	1.91	0.52
1:A:296:MET:HE3	1:A:296:MET:HA	1.90	0.52
1:A:449:TYR:HB2	1:A:462:ILE:HD12	1.92	0.52
2:A:900:FHP:H133	2:A:900:FHP:C8	2.19	0.52
1:A:394:TYR:CZ	1:A:461:GLY:HA2	2.44	0.51
1:A:514:ARG:CA	1:A:517:GLU:OE1	2.58	0.51
1:A:34:ILE:HG23	1:A:34:ILE:O	2.10	0.51
1:A:23:SER:HA	1:A:24:LEU:HD23	1.92	0.51
1:A:23:SER:O	1:A:25:TRP:N	2.45	0.50
1:A:339:TYR:CE2	1:A:343:LEU:HD11	2.47	0.49
1:A:462:ILE:HG23	1:A:476:ALA:HB1	1.94	0.49
1:A:514:ARG:C	1:A:517:GLU:OE1	2.56	0.48
1:A:395:LEU:O	1:A:399:LEU:HG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:O	1:A:294:ILE:HG13	2.13	0.48
1:A:221:LYS:HD2	1:A:226:LEU:HD22	1.95	0.47
1:A:446:THR:HA	1:A:462:ILE:HD11	1.97	0.47
1:A:264:ARG:N	1:A:302:ASP:OD2	2.45	0.47
1:A:354:SER:HA	1:A:359:SER:OG	2.14	0.47
2:A:900:FHP:H52	2:A:900:FHP:H151	1.82	0.45
1:A:53:THR:HA	1:A:56:MET:HE3	1.98	0.45
1:A:296:MET:CE	1:A:299:ILE:HD12	2.47	0.45
1:A:21:SER:HA	1:A:22:PRO:HD3	1.71	0.45
1:A:391:VAL:HG21	1:A:469:TYR:HE2	1.82	0.43
1:A:449:TYR:O	1:A:449:TYR:CD1	2.72	0.43
1:A:132:GLU:O	1:A:133:ASN:HB2	2.18	0.43
1:A:369:MET:O	1:A:373:VAL:HG23	2.19	0.43
1:A:469:TYR:CZ	1:A:479:LYS:NZ	2.87	0.43
1:A:473:THR:O	1:A:477:MET:HG3	2.19	0.43
1:A:260:LEU:CD2	1:A:334:TYR:HB2	2.50	0.42
1:A:533:VAL:O	1:A:533:VAL:CG2	2.65	0.42
1:A:25:TRP:CH2	1:A:535:LYS:HG3	2.55	0.42
1:A:403:THR:O	1:A:406:TYR:HB3	2.20	0.42
1:A:368:ARG:O	1:A:372:VAL:HG23	2.19	0.42
1:A:284:SER:O	1:A:288:VAL:HG23	2.20	0.41
1:A:463:GLU:HA	1:A:466:MET:HE2	2.01	0.41
1:A:477:MET:O	1:A:481:GLN:HG2	2.20	0.41
1:A:208:ARG:HD3	1:A:233:PHE:CZ	2.55	0.41
1:A:359:SER:O	1:A:362:VAL:CG2	2.63	0.41
1:A:463:GLU:HA	1:A:466:MET:CE	2.51	0.41
1:A:332:PRO:O	1:A:336:LYS:HG3	2.22	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	512/548 (93%)	489 (96%)	18 (4%)	5 (1%)	12 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	22	PRO
1	A	307	TYR
1	A	24	LEU
1	A	35	ASP

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	463/489 (95%)	454 (98%)	9 (2%)	50 61

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	33	SER
1	A	35	ASP
1	A	124	GLU
1	A	247	VAL
1	A	278	TYR
1	A	305	ASP
1	A	460	THR
1	A	497	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	97	GLN

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Mol	Chain	Res	Type
1	A	100	ASN
1	A	102	ASN
1	A	149	ASN
1	A	155	HIS
1	A	189	GLN
1	A	360	HIS
1	A	540	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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	$\# Z > 2$
2	FHP	A	900	-	17,19,19	1.28	3 (17%)	21,25,25	1.89	7 (33%)

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
2	FHP	A	900	-	-	5/18/22/22	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	FHP	PA-O3A	-2.59	1.50	1.54
2	A	900	FHP	PA-O2A	-2.26	1.51	1.54
2	A	900	FHP	C6-C7	2.00	1.37	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	FHP	O1A-PA-C1	-4.84	100.50	113.03
2	A	900	FHP	C15-C3-C4	3.00	120.43	115.23
2	A	900	FHP	O3A-PA-O2A	2.81	115.22	107.58
2	A	900	FHP	C5-C6-C7	-2.62	121.62	127.62
2	A	900	FHP	C14-C7-C8	2.46	119.50	115.23
2	A	900	FHP	C13-C11-C12	2.26	119.80	114.59
2	A	900	FHP	C9-C10-C11	-2.07	120.75	127.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	FHP	O1-C1-C2-C3
2	A	900	FHP	C2-C3-C4-C5
2	A	900	FHP	C15-C3-C4-C5
2	A	900	FHP	C11-C10-C9-C8
2	A	900	FHP	C7-C8-C9-C10

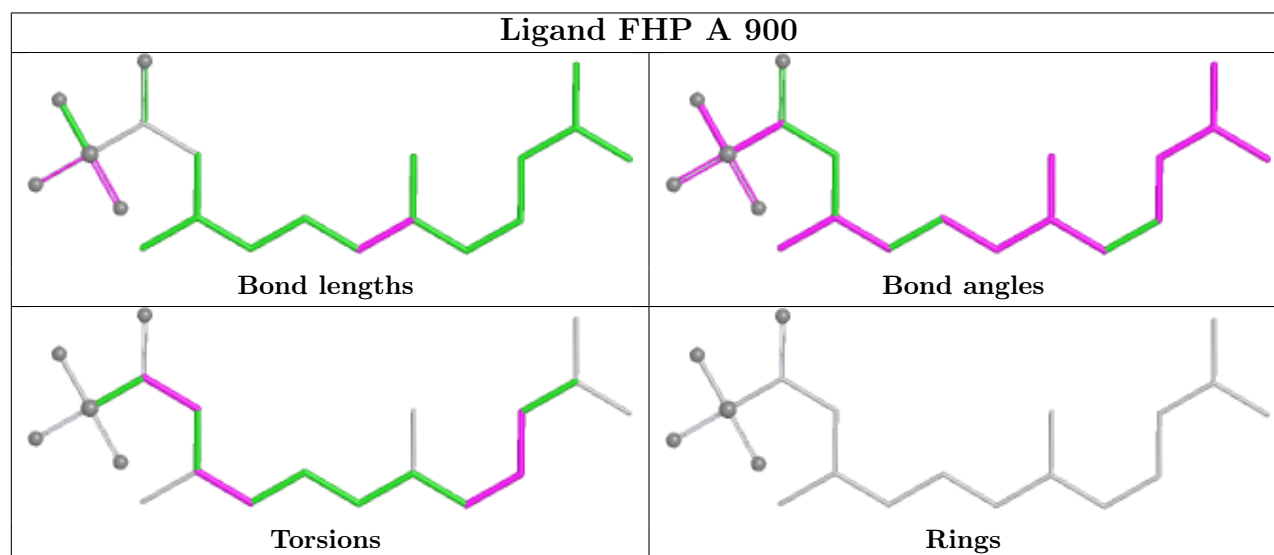
There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	FHP	17	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.



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	516/548 (94%)	1.76	200 (38%) 1 0	29, 55, 98, 102	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	GLU	9.7
1	A	354	SER	9.0
1	A	257	VAL	8.4
1	A	35	ASP	8.0
1	A	306	ALA	7.5
1	A	258	THR	7.3
1	A	458	ILE	7.2
1	A	451	VAL	7.2
1	A	456	GLY	6.7
1	A	452	GLU	6.5
1	A	533	VAL	6.3
1	A	259	THR	6.2
1	A	548	ILE	6.1
1	A	309	THR	6.0
1	A	356	ALA	5.8
1	A	255	ASP	5.7
1	A	457	GLN	5.5
1	A	101	CYS	5.5
1	A	99	SER	5.5
1	A	100	ASN	5.5
1	A	24	LEU	5.5
1	A	311	LYS	5.5
1	A	325	ILE	5.5
1	A	449	TYR	5.4
1	A	59	ALA	5.4
1	A	21	SER	5.3
1	A	459	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	310	VAL	5.1
1	A	355	SER	5.0
1	A	326	ASN	5.0
1	A	27	ASP	5.0
1	A	26	GLY	4.9
1	A	332	PRO	4.9
1	A	260	LEU	4.7
1	A	22	PRO	4.7
1	A	460	THR	4.6
1	A	471	ILE	4.6
1	A	124	GLU	4.6
1	A	448	THR	4.6
1	A	318	ASP	4.5
1	A	312	GLU	4.5
1	A	467	ARG	4.5
1	A	328	ILE	4.5
1	A	380	SER	4.4
1	A	453	LYS	4.4
1	A	450	GLU	4.4
1	A	338	SER	4.3
1	A	34	ILE	4.3
1	A	31	SER	4.3
1	A	357	GLY	4.3
1	A	334	TYR	4.2
1	A	520	TYR	4.2
1	A	421	GLN	4.2
1	A	98	ASN	4.2
1	A	37	GLN	4.1
1	A	30	LEU	4.1
1	A	359	SER	4.1
1	A	23	SER	4.1
1	A	424	GLU	4.1
1	A	253	ASP	4.0
1	A	262	TYR	3.9
1	A	455	ARG	3.9
1	A	518	VAL	3.8
1	A	319	ALA	3.8
1	A	102	ASN	3.8
1	A	33	SER	3.8
1	A	62	MET	3.8
1	A	263	ALA	3.8
1	A	254	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	476	ALA	3.7
1	A	132	GLU	3.7
1	A	331	LEU	3.6
1	A	462	ILE	3.6
1	A	63	LYS	3.6
1	A	60	THR	3.5
1	A	470	GLY	3.5
1	A	89	ASP	3.5
1	A	131	ASP	3.5
1	A	261	PRO	3.5
1	A	315	ALA	3.5
1	A	454	SER	3.5
1	A	93	GLN	3.5
1	A	308	GLY	3.4
1	A	468	ASP	3.4
1	A	469	TYR	3.4
1	A	25	TRP	3.3
1	A	336	LYS	3.3
1	A	130	GLN	3.3
1	A	329	ASP	3.3
1	A	351	LYS	3.3
1	A	219	GLN	3.3
1	A	474	LYS	3.3
1	A	51	GLU	3.3
1	A	307	TYR	3.3
1	A	485	GLU	3.2
1	A	36	ASN	3.2
1	A	166	ASP	3.2
1	A	128	LYS	3.1
1	A	55	ASN	3.1
1	A	316	TYR	3.1
1	A	363	CYS	3.1
1	A	195	GLU	3.0
1	A	339	TYR	3.0
1	A	317	THR	3.0
1	A	163	ILE	3.0
1	A	85	LYS	3.0
1	A	32	PHE	3.0
1	A	256	PHE	3.0
1	A	482	ASN	2.9
1	A	360	HIS	2.9
1	A	134	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	305	ASP	2.9
1	A	464	CYS	2.9
1	A	265	ASP	2.9
1	A	335	MET	2.9
1	A	461	GLY	2.8
1	A	547	LYS	2.8
1	A	478	ALA	2.8
1	A	252	LYS	2.8
1	A	340	LYS	2.8
1	A	127	SER	2.8
1	A	187	ARG	2.8
1	A	133	ASN	2.7
1	A	392	SER	2.7
1	A	58	LEU	2.7
1	A	391	VAL	2.7
1	A	251	TRP	2.7
1	A	264	ARG	2.7
1	A	343	LEU	2.7
1	A	362	VAL	2.6
1	A	322	ARG	2.6
1	A	516	VAL	2.6
1	A	246	GLN	2.6
1	A	333	ASP	2.6
1	A	473	THR	2.6
1	A	323	TRP	2.6
1	A	295	SER	2.6
1	A	502	SER	2.5
1	A	330	ARG	2.5
1	A	358	ARG	2.5
1	A	96	ASN	2.5
1	A	519	THR	2.5
1	A	481	GLN	2.5
1	A	173	ILE	2.5
1	A	61	GLY	2.5
1	A	92	ASP	2.5
1	A	390	PRO	2.5
1	A	40	GLU	2.4
1	A	381	THR	2.4
1	A	324	ASP	2.4
1	A	28	GLN	2.4
1	A	266	ARG	2.4
1	A	327	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	273	TRP	2.4
1	A	477	MET	2.4
1	A	42	TYR	2.4
1	A	301	ASP	2.4
1	A	442	VAL	2.4
1	A	120	ASN	2.4
1	A	299	ILE	2.4
1	A	353	LEU	2.3
1	A	347	LYS	2.3
1	A	416	LYS	2.3
1	A	313	LEU	2.3
1	A	29	PHE	2.3
1	A	84	GLU	2.3
1	A	444	ASP	2.2
1	A	350	GLU	2.2
1	A	387	TYR	2.2
1	A	83	PHE	2.2
1	A	97	GLN	2.2
1	A	220	SER	2.2
1	A	337	ILE	2.2
1	A	384	ILE	2.2
1	A	397	ASN	2.2
1	A	377	ASN	2.2
1	A	378	VAL	2.2
1	A	352	GLU	2.2
1	A	465	CYS	2.2
1	A	302	ASP	2.1
1	A	463	GLU	2.1
1	A	41	LYS	2.1
1	A	135	LYS	2.1
1	A	38	VAL	2.1
1	A	53	THR	2.1
1	A	248	SER	2.1
1	A	138	GLU	2.1
1	A	95	TYR	2.1
1	A	344	ASP	2.1
1	A	250	TRP	2.1
1	A	419	THR	2.1
1	A	65	ALA	2.1
1	A	479	LYS	2.1
1	A	137	LYS	2.0
1	A	503	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	379	GLU	2.0
1	A	447	ALA	2.0
1	A	321	GLN	2.0
1	A	417	SER	2.0
1	A	241	LYS	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](#)

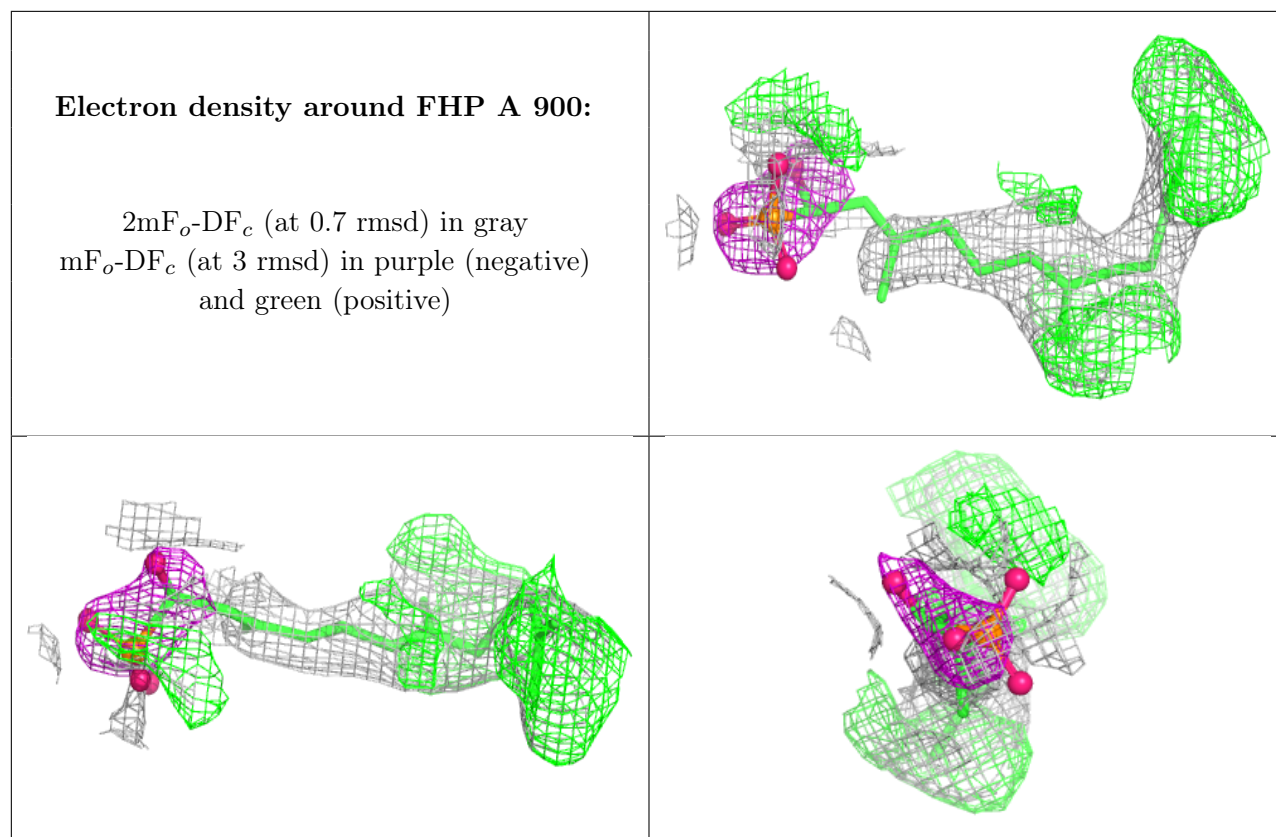
There are no oligosaccharides in this entry.

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, 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
2	FHP	A	900	20/20	0.39	0.47	36,58,70,75	20

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



6.5 Other polymers [i](#)

There are no such residues in this entry.