Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 09:59 PM EST

PDB ID	:	1N95
Title	:	Aryl Tetrahydrophyridine Inhbitors of Farnesyltranferase: Glycine, Phenylalanine and Histidine Derivatives
Authors	:	Gwaltney II, S.L.; O'Conner, S.J.; Nelson, L.T.; Sullivan, G.M.; Imade, H.; Wang, W.; Hasvold, L.; Li, Q.; Cohen, J.; Gu, W.Z.
Deposited on	:	2002-11-22
Resolution	:	2.30 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 (i)) were used in the production of this report:

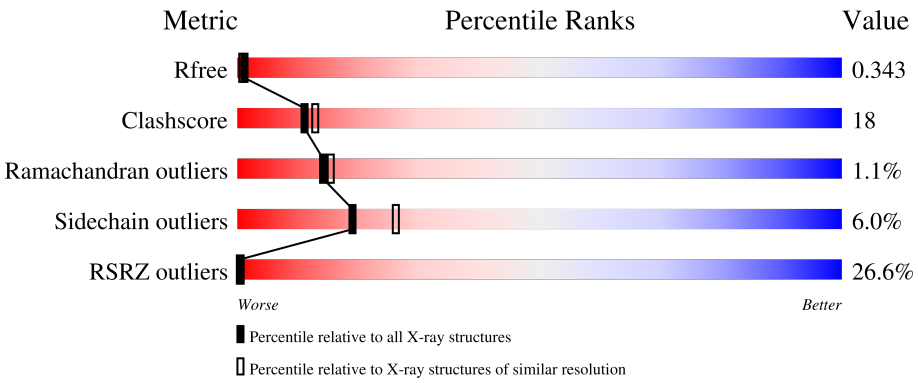
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	315	32% 63% 32%
2	B	402	22% 60% 36%

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
4	HFP	B	501	X	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5873 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 Protein farnesyltransferase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	312	2660	1695	465	495	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	THR	ILE	conflict	UNP Q04631

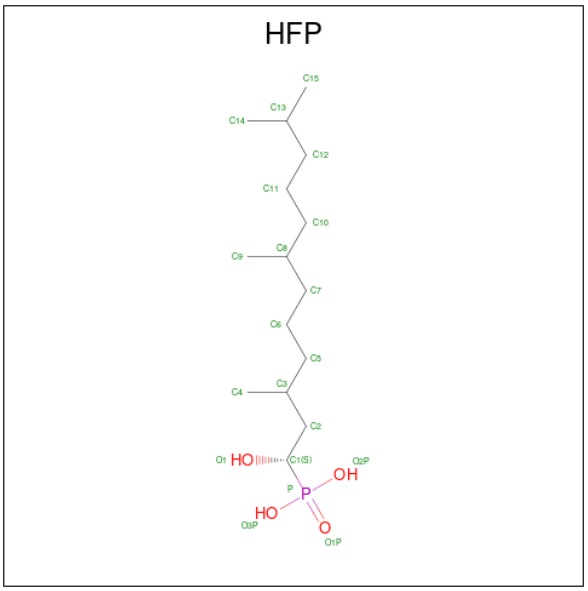
- Molecule 2 is a protein called Protein farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	401	3154	2016	543	572	23	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

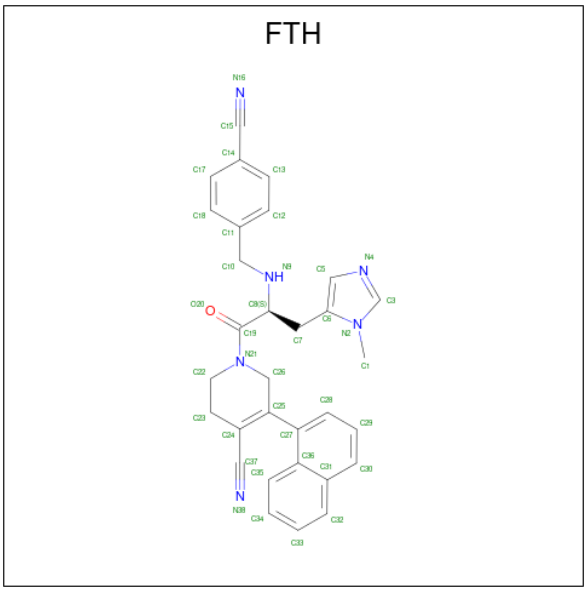
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	1	1	1	0	0

- Molecule 4 is ALPHA-HYDROXYFARNESYLPHOSPHONIC ACID (three-letter code: HFP) (formula: $C_{15}H_{33}O_4P$).



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

- Molecule 5 is 1-[2-(4-CYANO-BENZYLAMINO)-3-(3-METHYL-3H-IMIDAZOL-4-YL)-PROPIONYL]-5-NAPHTHALEN-1-YL-1,2,3,6-TETRAHYDRO-PYRIDINE-4-CARBONITRILE (three-letter code: FTH) (formula: $C_{31}H_{28}N_6O$).



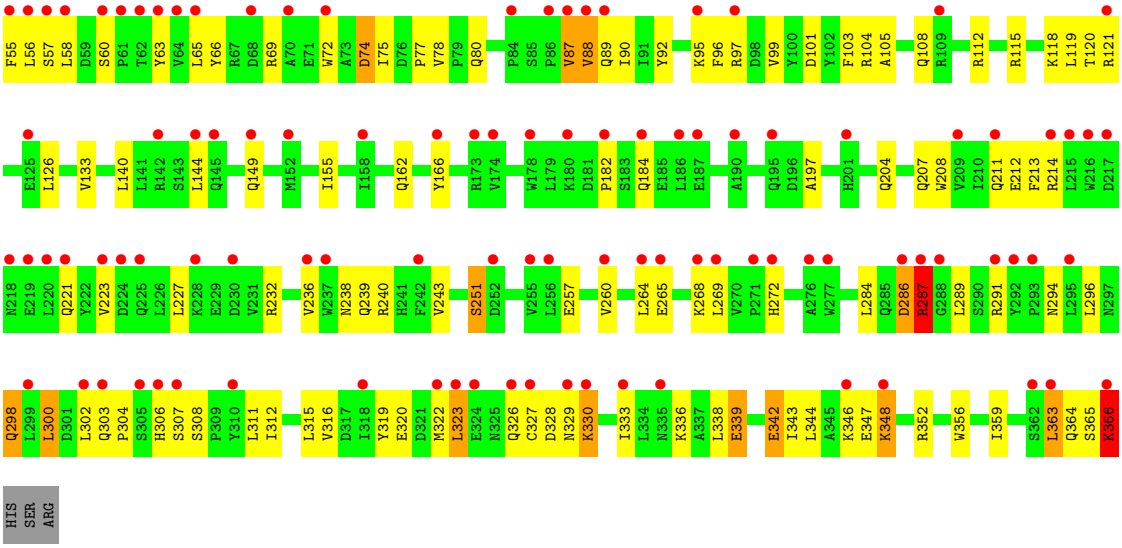
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	38	31	6	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

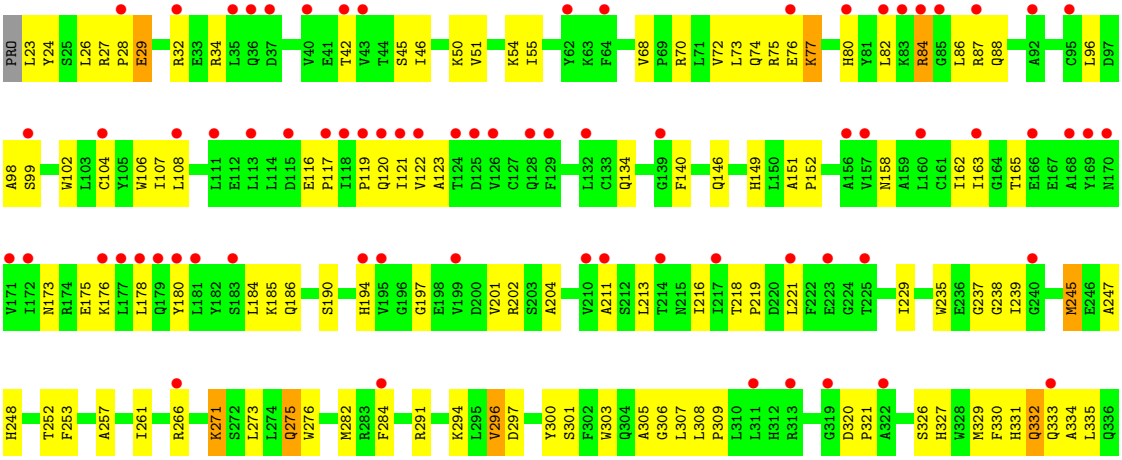
• Molecule 1: Protein farnesyltransferase alpha subunit

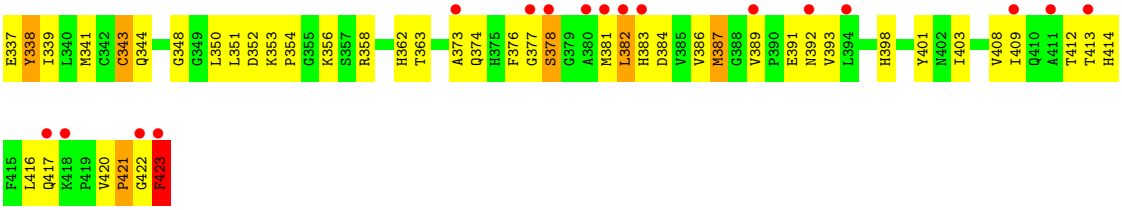
Chain A:



• Molecule 2: Protein farnesyltransferase beta subunit

Chain B:




E337 Y338 I339 L340 M341 C342 C343 Q344
G348 G349 L350 L351 D352 K353 P354 G355 K356 S357 R358
H362 T363
A373 Q374 H375 F376 G377 S378 G379 A380 M381 L382 H383 D384 V385 V386 M387 G388 V389 P390 E391 N392 V393 L394
H398
Y401 N402 I403
V408 I409 Q410 A411 T412 T413 H414
F415 L416 Q417 K418 P419 V420 P421 G422 F423

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	171.13Å 171.13Å 69.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.59 – 2.30 43.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.59-2.30) 83.5 (43.59-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.33 (at 2.29Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.337 , 0.358 0.323 , 0.343	Depositor DCC
R_{free} test set	5035 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 26.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	5873	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HFP, ZN, FTH

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	0.59	1/2725 (0.0%)	0.83	4/3700 (0.1%)
2	B	0.60	3/3239 (0.1%)	0.83	1/4397 (0.0%)
All	All	0.60	4/5964 (0.1%)	0.83	5/8097 (0.1%)

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
2	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	343	CYS	CB-SG	-7.00	1.70	1.82
2	B	423	PHE	C-O	6.61	1.35	1.23
2	B	423	PHE	C-OXT	6.03	1.34	1.23
1	A	366	LYS	CA-CB	6.00	1.67	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	423	PHE	CA-C-O	23.35	169.13	120.10
1	A	366	LYS	CA-C-O	15.64	152.94	120.10
1	A	287	ARG	NE-CZ-NH1	-14.37	113.11	120.30
1	A	74	ASP	CB-CG-OD1	-9.70	109.57	118.30
1	A	74	ASP	CB-CG-OD2	5.60	123.34	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	338	TYR	Sidechain

5.2 Too-close contacts (i)

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	2660	0	2585	82	3
2	B	3154	0	3085	123	2
3	B	1	0	0	0	0
4	B	20	0	28	10	0
5	B	38	0	28	14	0
All	All	5873	0	5726	209	3

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 18.

All (209) 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)
2:B:245:MET:HE3	2:B:245:MET:HA	1.52	0.91
2:B:77:LYS:HE3	2:B:77:LYS:HA	1.53	0.90
2:B:271:LYS:HA	2:B:271:LYS:HE3	1.54	0.87
2:B:84:ARG:HH22	2:B:88:GLN:HG2	1.40	0.83
2:B:218:THR:HB	2:B:219:PRO:HD2	1.62	0.81
2:B:185:LYS:HE3	2:B:221:LEU:O	1.82	0.79
1:A:322:MET:HE3	1:A:333:ILE:HD13	1.65	0.79
2:B:106:TRP:CH2	5:B:1001:FTH:HC13	2.20	0.76
1:A:312:ILE:O	1:A:316:VAL:HG23	1.86	0.75
2:B:178:LEU:HD12	2:B:421:PRO:HB2	1.68	0.74
2:B:116:GLU:HB3	2:B:117:PRO:HD2	1.70	0.73
1:A:287:ARG:HD3	1:A:291:ARG:HD3	1.71	0.72
2:B:84:ARG:NH2	2:B:88:GLN:HG2	2.05	0.71
2:B:178:LEU:HG	2:B:216:ILE:HB	1.72	0.71
2:B:338:TYR:CE2	2:B:343:CYS:SG	2.86	0.69
2:B:151:ALA:HB3	2:B:152:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:CYS:O	1:A:330:LYS:HB3	1.93	0.67
2:B:73:LEU:O	2:B:75:ARG:N	2.28	0.66
2:B:253:PHE:HA	2:B:307:LEU:HD21	1.78	0.66
2:B:82:LEU:HD21	2:B:363:THR:HG21	1.78	0.66
1:A:365:SER:HB2	1:A:366:LYS:HD3	1.77	0.66
1:A:268:LYS:HE2	1:A:302:LEU:HD11	1.79	0.65
1:A:344:LEU:HD23	1:A:348:LYS:HB3	1.78	0.65
1:A:343:ILE:HG22	1:A:348:LYS:HB2	1.78	0.64
1:A:303:GLN:O	1:A:307:SER:HB2	1.98	0.63
1:A:312:ILE:HD12	1:A:348:LYS:HG2	1.79	0.63
1:A:302:LEU:HD22	1:A:306:HIS:CD2	2.33	0.63
2:B:72:VAL:HG22	2:B:389:VAL:HG21	1.80	0.63
2:B:335:LEU:O	2:B:339:ILE:HG13	1.99	0.63
2:B:96:LEU:HD11	5:B:1001:FTH:C14	2.29	0.63
2:B:301:SER:O	2:B:305:ALA:HB3	1.98	0.63
1:A:223:VAL:HG11	1:A:240:ARG:HB2	1.81	0.62
2:B:327:HIS:HB3	2:B:332:GLN:HE22	1.64	0.62
2:B:73:LEU:HD12	2:B:344:GLN:OE1	1.99	0.62
2:B:353:LYS:HB2	2:B:354:PRO:HD2	1.81	0.61
1:A:80:GLN:HB2	1:A:104:ARG:CZ	2.31	0.61
2:B:51:VAL:HA	2:B:54:LYS:HE2	1.83	0.59
2:B:308:LEU:HD13	2:B:330:PHE:HB3	1.84	0.59
1:A:359:ILE:O	1:A:363:LEU:HB2	2.02	0.59
2:B:239:ILE:HB	2:B:252:THR:HA	1.85	0.59
2:B:96:LEU:HD11	5:B:1001:FTH:C15	2.32	0.59
2:B:73:LEU:H	2:B:392:ASN:ND2	2.00	0.58
2:B:352:ASP:HB3	2:B:356:LYS:HG3	1.86	0.58
1:A:347:GLU:HG2	1:A:348:LYS:HE3	1.85	0.58
2:B:180:TYR:CZ	2:B:184:LEU:HD11	2.38	0.58
4:B:501:HFP:H52	5:B:1001:FTH:H231	1.85	0.58
1:A:208:TRP:NE1	1:A:212:GLU:HG3	2.20	0.57
2:B:104:CYS:O	2:B:108:LEU:HB2	2.05	0.57
2:B:308:LEU:CD1	2:B:330:PHE:HB3	2.35	0.57
2:B:282:MET:CG	2:B:296:VAL:HG13	2.34	0.57
4:B:501:HFP:C5	5:B:1001:FTH:H231	2.35	0.57
2:B:98:ALA:HA	2:B:146:GLN:HE22	1.69	0.56
1:A:342:GLU:OE1	1:A:346:LYS:HE3	2.06	0.56
1:A:366:LYS:HD3	1:A:366:LYS:N	2.21	0.56
1:A:55:PHE:HB2	1:A:118:LYS:HD3	1.87	0.56
1:A:104:ARG:O	1:A:108:GLN:HB2	2.05	0.55
1:A:286:ASP:O	1:A:287:ARG:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TYR:HD2	1:A:322:MET:HE2	1.71	0.55
1:A:87:VAL:O	1:A:88:VAL:C	2.43	0.55
1:A:90:ILE:HB	1:A:92:TYR:CE2	2.42	0.55
1:A:149:GLN:HE22	1:A:184:GLN:HE22	1.54	0.55
2:B:282:MET:HG3	2:B:296:VAL:HG13	1.89	0.55
1:A:338:LEU:HD11	1:A:364:GLN:HE22	1.72	0.55
2:B:72:VAL:HG22	2:B:389:VAL:CG2	2.37	0.55
2:B:75:ARG:NH2	2:B:391:GLU:O	2.40	0.54
2:B:257:ALA:O	2:B:261:ILE:HG13	2.07	0.54
2:B:386:VAL:HG21	2:B:393:VAL:HB	1.89	0.54
1:A:294:ASN:O	1:A:298:GLN:HG2	2.06	0.54
2:B:374:GLN:O	2:B:384:ASP:HA	2.08	0.54
2:B:398:HIS:CD2	2:B:408:VAL:HG11	2.42	0.54
2:B:326:SER:O	2:B:383:HIS:HB3	2.08	0.53
1:A:356:TRP:HA	1:A:356:TRP:CE3	2.44	0.53
2:B:362:HIS:CE1	5:B:1001:FTH:N4	2.77	0.53
2:B:202:ARG:HD3	5:B:1001:FTH:N38	2.23	0.53
2:B:84:ARG:HH22	2:B:88:GLN:CG	2.17	0.53
1:A:75:ILE:HD11	1:A:115:ARG:CZ	2.39	0.53
2:B:86:LEU:HB2	2:B:107:ILE:HG21	1.90	0.53
2:B:381:MET:O	2:B:382:LEU:HD22	2.09	0.53
2:B:337:GLU:HB3	2:B:341:MET:HE3	1.91	0.52
1:A:287:ARG:HD3	1:A:287:ARG:O	2.09	0.52
4:B:501:HFP:H112	5:B:1001:FTH:C28	2.39	0.52
2:B:50:LYS:O	2:B:54:LYS:HG3	2.09	0.52
2:B:398:HIS:CD2	2:B:408:VAL:HG21	2.44	0.52
1:A:96:PHE:HA	1:A:126:LEU:HD13	1.93	0.51
2:B:186:GLN:HB2	2:B:190:SER:O	2.10	0.51
1:A:223:VAL:HG13	1:A:236:VAL:HG12	1.93	0.51
2:B:46:ILE:HG22	2:B:50:LYS:HE3	1.93	0.51
1:A:72:TRP:CE3	1:A:75:ILE:HD12	2.45	0.51
2:B:76:GLU:O	2:B:80:HIS:ND1	2.44	0.51
2:B:158:ASN:O	2:B:162:ILE:HG13	2.12	0.50
2:B:414:HIS:O	2:B:417:GLN:HG2	2.11	0.50
2:B:348:GLY:O	2:B:358:ARG:HD2	2.11	0.50
1:A:302:LEU:HD22	1:A:306:HIS:HD2	1.74	0.50
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.46	0.50
1:A:296:LEU:O	1:A:300:LEU:HB2	2.11	0.50
2:B:275:GLN:HE21	2:B:276:TRP:N	2.10	0.50
1:A:78:VAL:HG23	1:A:105:ALA:HB2	1.94	0.50
1:A:328:ASP:O	1:A:329:ASN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:MET:HA	2:B:245:MET:CE	2.35	0.50
2:B:344:GLN:HA	2:B:350:LEU:HD13	1.93	0.50
2:B:297:ASP:HB3	2:B:300:TYR:HD1	1.76	0.49
2:B:412:THR:O	2:B:416:LEU:HB2	2.12	0.49
2:B:23:LEU:O	2:B:27:ARG:HG3	2.12	0.49
2:B:389:VAL:HG12	2:B:391:GLU:HB2	1.94	0.48
2:B:350:LEU:HB2	2:B:363:THR:HA	1.95	0.48
1:A:182:PRO:HG3	1:A:213:PHE:CD2	2.49	0.48
1:A:227:LEU:HG	1:A:236:VAL:CG1	2.44	0.48
1:A:89:GLN:OE1	2:B:87:ARG:NH2	2.47	0.48
2:B:73:LEU:H	2:B:392:ASN:HD21	1.62	0.48
2:B:23:LEU:HD12	2:B:26:LEU:CD1	2.44	0.48
1:A:238:ASN:HA	2:B:235:TRP:CZ2	2.50	0.47
2:B:326:SER:HB2	2:B:383:HIS:CD2	2.49	0.47
2:B:121:ILE:N	2:B:121:ILE:HD12	2.30	0.47
1:A:311:LEU:O	1:A:315:LEU:HG	2.14	0.47
1:A:312:ILE:HG22	1:A:344:LEU:HD11	1.96	0.47
2:B:216:ILE:HG22	2:B:421:PRO:CD	2.44	0.47
2:B:308:LEU:HD22	2:B:329:MET:HB2	1.97	0.47
2:B:51:VAL:O	2:B:55:ILE:HG12	2.15	0.47
2:B:119:PRO:O	2:B:122:VAL:HG12	2.15	0.46
2:B:376:PHE:CZ	2:B:378:SER:HB2	2.50	0.46
2:B:134:GLN:HB2	2:B:140:PHE:CE2	2.51	0.46
1:A:92:TYR:HB2	1:A:97:ARG:HG3	1.98	0.46
2:B:55:ILE:HD13	2:B:354:PRO:HG3	1.98	0.46
1:A:80:GLN:HB2	1:A:104:ARG:NH2	2.31	0.45
2:B:108:LEU:O	2:B:162:ILE:HG21	2.17	0.45
1:A:312:ILE:CD1	1:A:348:LYS:HG2	2.45	0.45
2:B:378:SER:HB3	2:B:381:MET:HG3	1.99	0.45
2:B:423:PHE:N	2:B:423:PHE:CD2	2.84	0.45
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.86	0.45
1:A:300:LEU:HD12	1:A:300:LEU:HA	1.81	0.45
2:B:306:GLY:O	2:B:309:PRO:HD2	2.17	0.45
2:B:218:THR:HB	2:B:219:PRO:CD	2.42	0.44
2:B:282:MET:HG2	2:B:296:VAL:HG13	1.99	0.44
2:B:213:LEU:HD23	2:B:412:THR:HG22	2.00	0.44
1:A:166:TYR:HE1	5:B:1001:FTH:H232	1.82	0.44
1:A:204:GLN:HA	2:B:245:MET:SD	2.58	0.44
1:A:239:GLN:O	1:A:243:VAL:HG23	2.18	0.44
2:B:420:VAL:O	2:B:422:GLY:N	2.50	0.44
1:A:58:LEU:O	1:A:95:LYS:NZ	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:O	1:A:144:LEU:HD21	2.18	0.44
2:B:248:HIS:CE1	4:B:501:HFP:H62	2.53	0.44
2:B:194:HIS:CD2	2:B:197:GLY:HA3	2.53	0.44
2:B:331:HIS:CD2	2:B:334:ALA:H	2.36	0.44
1:A:72:TRP:CZ3	1:A:75:ILE:HD12	2.53	0.43
1:A:77:PRO:HB2	1:A:101:ASP:HB3	2.00	0.43
2:B:173:ASN:CG	2:B:176:LYS:HB2	2.39	0.43
1:A:316:VAL:O	1:A:320:GLU:HG3	2.17	0.43
1:A:319:TYR:CE1	1:A:336:LYS:HG3	2.53	0.43
2:B:237:GLY:O	2:B:273:LEU:HA	2.19	0.43
2:B:303:TRP:CH2	4:B:501:HFP:H121	2.53	0.43
4:B:501:HFP:H112	5:B:1001:FTH:HC28	2.00	0.43
1:A:339:GLU:O	1:A:343:ILE:HG13	2.18	0.43
2:B:46:ILE:O	2:B:50:LYS:HG3	2.18	0.43
2:B:398:HIS:HD2	2:B:408:VAL:HG11	1.83	0.43
2:B:376:PHE:CG	2:B:377:GLY:N	2.86	0.43
2:B:122:VAL:HG13	2:B:123:ALA:N	2.33	0.43
2:B:149:HIS:HB3	2:B:152:PRO:HD2	1.99	0.43
2:B:99:SER:O	2:B:102:TRP:HB2	2.19	0.43
2:B:163:ILE:HG22	2:B:165:THR:HG23	2.00	0.43
1:A:260:VAL:HG21	1:A:284:LEU:HD21	2.00	0.43
2:B:24:TYR:HB2	2:B:333:GLN:CD	2.39	0.43
4:B:501:HFP:H52	5:B:1001:FTH:C23	2.49	0.43
2:B:175:GLU:CD	2:B:175:GLU:H	2.22	0.43
1:A:99:VAL:HG13	1:A:119:LEU:CD1	2.49	0.43
1:A:155:ILE:HD12	1:A:155:ILE:HA	1.88	0.42
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.91	0.42
2:B:121:ILE:HD12	2:B:121:ILE:H	1.83	0.42
1:A:312:ILE:HB	1:A:344:LEU:HD21	2.02	0.42
2:B:204:ALA:HB1	2:B:229:ILE:HD11	2.01	0.42
2:B:409:ILE:O	2:B:413:THR:HG23	2.19	0.42
2:B:403:ILE:HG13	2:B:408:VAL:HG23	2.00	0.42
1:A:232:ARG:NH1	2:B:42:THR:HG23	2.34	0.42
2:B:331:HIS:HD2	2:B:334:ALA:H	1.66	0.42
2:B:408:VAL:O	2:B:412:THR:HG23	2.20	0.42
2:B:29:GLU:O	2:B:32:ARG:HD2	2.20	0.42
2:B:238:GLY:HA3	2:B:247:ALA:HB1	2.01	0.42
4:B:501:HFP:H21	5:B:1001:FTH:H231	2.01	0.42
2:B:173:ASN:OD1	2:B:175:GLU:HG2	2.19	0.42
2:B:333:GLN:HG3	2:B:387:MET:CE	2.49	0.42
2:B:291:ARG:HB2	2:B:294:LYS:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HA	1:A:140:LEU:HD21	2.02	0.42
2:B:218:THR:CB	2:B:219:PRO:HD2	2.44	0.42
1:A:322:MET:HE3	1:A:333:ILE:CD1	2.43	0.41
1:A:99:VAL:HG13	1:A:119:LEU:HD11	2.02	0.41
1:A:103:PHE:HE1	1:A:120:THR:HG22	1.85	0.41
2:B:335:LEU:HD23	2:B:373:ALA:HB2	2.02	0.41
1:A:57:SER:O	1:A:63:TYR:HD1	2.04	0.41
1:A:272:HIS:CD2	1:A:308:SER:HB3	2.56	0.41
1:A:287:ARG:CD	1:A:291:ARG:HD3	2.45	0.41
2:B:294:LYS:HD2	2:B:294:LYS:HA	1.94	0.41
4:B:501:HFP:H112	5:B:1001:FTH:C29	2.50	0.41
2:B:320:ASP:HA	2:B:321:PRO:HD3	1.70	0.41
1:A:302:LEU:HB3	1:A:306:HIS:HB2	2.02	0.41
4:B:501:HFP:H61	5:B:1001:FTH:H231	2.02	0.41
1:A:338:LEU:HD21	1:A:363:LEU:HB3	2.01	0.41
1:A:58:LEU:HD22	1:A:95:LYS:HE3	2.02	0.41
2:B:122:VAL:CG1	2:B:123:ALA:N	2.84	0.41
2:B:211:ALA:HA	2:B:216:ILE:CG1	2.51	0.41
2:B:213:LEU:HG	2:B:401:TYR:CE2	2.56	0.41
1:A:65:LEU:O	1:A:69:ARG:HG3	2.21	0.41
1:A:207:GLN:O	1:A:211:GLN:HB2	2.21	0.40
1:A:66:TYR:CZ	1:A:119:LEU:HD13	2.55	0.40
1:A:72:TRP:CZ2	1:A:115:ARG:HD2	2.57	0.40
1:A:328:ASP:O	1:A:329:ASN:CB	2.68	0.40
1:A:363:LEU:HD12	1:A:363:LEU:HA	1.90	0.40
2:B:403:ILE:HG13	2:B:408:VAL:CG2	2.52	0.40
1:A:323:LEU:HD13	1:A:333:ILE:HG21	2.02	0.40
2:B:27:ARG:HA	2:B:28:PRO:HD3	1.87	0.40
2:B:34:ARG:HD2	2:B:284:PHE:CE1	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:SER:OG	1:A:257:GLU:OE1[6_555]	2.08	0.12
1:A:251:SER:CB	2:B:120:GLN:OE1[2_655]	2.17	0.03
1:A:74:ASP:O	2:B:84:ARG:NH2[4_665]	2.19	0.01

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	310/315 (98%)	278 (90%)	27 (9%)	5 (2%)	9 9
2	B	399/402 (99%)	370 (93%)	26 (6%)	3 (1%)	19 23
All	All	709/717 (99%)	648 (91%)	53 (8%)	8 (1%)	14 15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ARG
2	B	74	GLN
1	A	326	GLN
2	B	378	SER
1	A	197	ALA
2	B	421	PRO
1	A	88	VAL
1	A	304	PRO

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	291/294 (99%)	270 (93%)	21 (7%)	14 18
2	B	338/339 (100%)	321 (95%)	17 (5%)	24 34
All	All	629/633 (99%)	591 (94%)	38 (6%)	19 26

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	87	VAL
1	A	121	ARG
1	A	162	GLN
1	A	214	ARG
1	A	221	GLN
1	A	251	SER
1	A	265	GLU
1	A	269	LEU
1	A	286	ASP
1	A	289	LEU
1	A	298	GLN
1	A	300	LEU
1	A	323	LEU
1	A	330	LYS
1	A	339	GLU
1	A	342	GLU
1	A	348	LYS
1	A	352	ARG
1	A	363	LEU
1	A	366	LYS
2	B	29	GLU
2	B	45	SER
2	B	68	VAL
2	B	70	ARG
2	B	77	LYS
2	B	84	ARG
2	B	201	VAL
2	B	245	MET
2	B	266	ARG
2	B	271	LYS
2	B	275	GLN
2	B	296	VAL
2	B	332	GLN
2	B	351	LEU
2	B	382	LEU
2	B	387	MET
2	B	423	PHE

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	80	GLN

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Mol	Chain	Res	Type
1	A	149	GLN
1	A	184	GLN
1	A	201	HIS
1	A	204	GLN
1	A	221	GLN
1	A	246	ASN
1	A	261	GLN
1	A	285	GLN
1	A	306	HIS
1	A	325	ASN
1	A	364	GLN
2	B	48	GLN
2	B	146	GLN
2	B	275	GLN
2	B	331	HIS
2	B	332	GLN
2	B	392	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HFP	B	501	-	17,19,19	1.93	4 (23%)	22,25,25	2.42	5 (22%)
5	FTH	B	1001	3	38,42,42	1.83	11 (28%)	47,58,58	1.94	7 (14%)

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
4	HFP	B	501	-	2/2/5/5	9/22/22/22	-
5	FTH	B	1001	3	-	12/23/38/38	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	HFP	C2-C3	-4.52	1.35	1.53
4	B	501	HFP	O1-C1	4.33	1.46	1.41
5	B	1001	FTH	C22-N21	-3.70	1.40	1.47
5	B	1001	FTH	C26-N21	3.29	1.51	1.46
5	B	1001	FTH	C28-C27	3.28	1.44	1.38
5	B	1001	FTH	C37-C24	3.13	1.46	1.43
4	B	501	HFP	C7-C8	-3.09	1.36	1.52
5	B	1001	FTH	C7-C6	2.96	1.55	1.50
5	B	1001	FTH	C13-C12	2.66	1.43	1.38
5	B	1001	FTH	C33-C32	2.64	1.42	1.36
5	B	1001	FTH	C8-C19	2.53	1.58	1.53
5	B	1001	FTH	C18-C17	2.24	1.42	1.38
5	B	1001	FTH	C18-C11	2.17	1.43	1.38
5	B	1001	FTH	C34-C35	2.08	1.41	1.36
4	B	501	HFP	P-O1P	-2.00	1.46	1.49

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	HFP	C3-C2-C1	8.20	123.53	115.21
5	B	1001	FTH	C22-C23-C24	7.13	118.40	109.14
5	B	1001	FTH	C25-C26-N21	6.19	115.27	109.62
5	B	1001	FTH	C26-N21-C22	3.63	122.15	114.47
5	B	1001	FTH	C23-C22-N21	3.48	116.43	110.54
4	B	501	HFP	C4-C3-C2	3.44	121.84	110.89
5	B	1001	FTH	C27-C25-C24	-3.37	119.70	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	HFP	C2-C3-C5	3.06	122.14	111.98
5	B	1001	FTH	C24-C37-N38	-3.05	171.88	176.99
5	B	1001	FTH	C1-N2-C6	2.78	128.14	124.44
4	B	501	HFP	C9-C8-C7	2.71	121.11	111.29
4	B	501	HFP	O1P-P-C1	-2.33	107.29	112.94

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	501	HFP	C8
4	B	501	HFP	C3

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	HFP	P-C1-C2-C3
4	B	501	HFP	C1-C2-C3-C4
4	B	501	HFP	C6-C7-C8-C9
5	B	1001	FTH	C8-C19-N21-C22
5	B	1001	FTH	C8-C19-N21-C26
5	B	1001	FTH	O20-C19-N21-C22
5	B	1001	FTH	O20-C19-N21-C26
4	B	501	HFP	C4-C3-C5-C6
4	B	501	HFP	C11-C12-C13-C14
4	B	501	HFP	O1-C1-C2-C3
5	B	1001	FTH	C7-C8-N9-C10
5	B	1001	FTH	C5-C6-C7-C8
5	B	1001	FTH	N2-C6-C7-C8
5	B	1001	FTH	N21-C19-C8-C7
5	B	1001	FTH	O20-C19-C8-N9
5	B	1001	FTH	C19-C8-N9-C10
4	B	501	HFP	C11-C10-C8-C9
5	B	1001	FTH	O20-C19-C8-C7
5	B	1001	FTH	N21-C19-C8-N9
4	B	501	HFP	C2-C3-C5-C6
4	B	501	HFP	C2-C1-P-O1P

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	HFP	10	0

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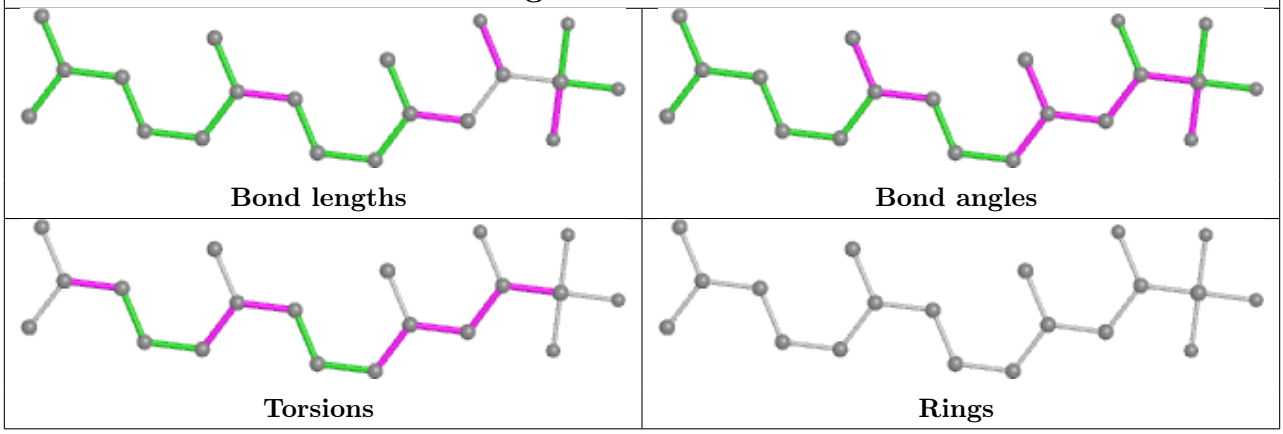
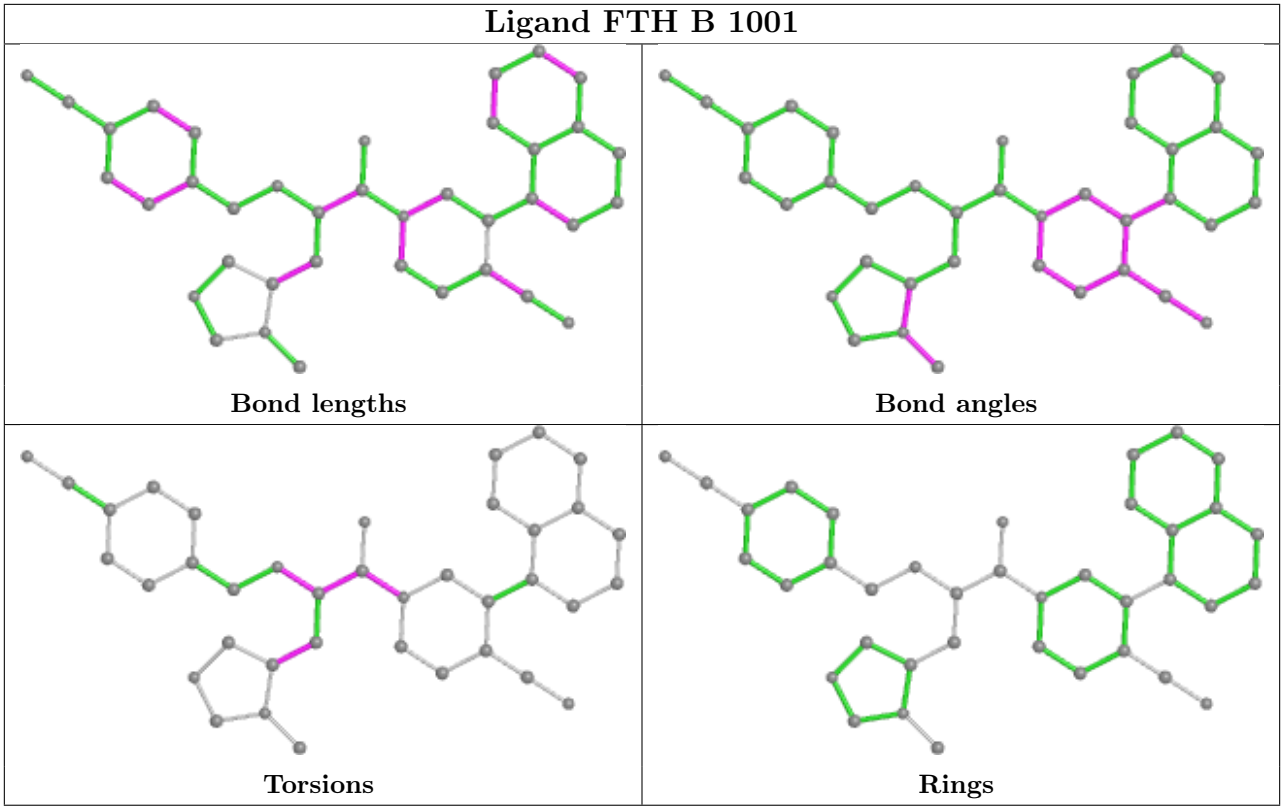
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	FTH	14	0

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 HFP B 501





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 (i)

6.1 Protein, DNA and RNA chains (i)

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	312/315 (99%)	1.67	100 (32%)	0	0	13, 41, 82, 100	0
2	B	401/402 (99%)	1.32	90 (22%)	0	1	11, 35, 72, 100	0
All	All	713/717 (99%)	1.47	190 (26%)	0	0	11, 37, 78, 100	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	117	PRO	12.7
1	A	55	PHE	12.4
2	B	423	PHE	11.8
1	A	56	LEU	9.4
1	A	61	PRO	7.3
1	A	326	GLN	7.2
2	B	40	VAL	7.1
2	B	122	VAL	7.1
2	B	378	SER	6.1
1	A	306	HIS	5.9
1	A	62	THR	5.9
2	B	422	GLY	5.9
1	A	291	ARG	5.6
2	B	84	ARG	5.6
2	B	87	ARG	5.2
1	A	366	LYS	5.1
2	B	80	HIS	5.0
2	B	128	GLN	5.0
1	A	87	VAL	4.7
1	A	58	LEU	4.7
1	A	57	SER	4.6
1	A	149	GLN	4.5
2	B	132	LEU	4.5
1	A	182	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	186	LEU	4.3
2	B	195	VAL	4.1
1	A	70	ALA	4.1
2	B	64	PHE	4.1
2	B	382	LEU	4.1
1	A	214	ARG	4.0
1	A	299	LEU	4.0
1	A	216	TRP	4.0
1	A	184	GLN	3.9
1	A	288	GLY	3.9
2	B	119	PRO	3.9
2	B	92	ALA	3.9
1	A	152	MET	3.9
1	A	255	VAL	3.8
2	B	179	GLN	3.7
1	A	221	GLN	3.7
2	B	409	ILE	3.6
1	A	292	TYR	3.6
1	A	323	LEU	3.6
2	B	322	ALA	3.6
1	A	295	LEU	3.5
1	A	225	GLN	3.5
2	B	76	GLU	3.5
1	A	303	GLN	3.5
2	B	83	LYS	3.4
1	A	63	TYR	3.4
2	B	221	LEU	3.4
1	A	180	LYS	3.4
2	B	389	VAL	3.3
1	A	173	ARG	3.3
1	A	217	ASP	3.3
2	B	120	GLN	3.3
1	A	64	VAL	3.3
1	A	174	VAL	3.3
1	A	145	GLN	3.3
2	B	211	ALA	3.2
1	A	215	LEU	3.2
1	A	65	LEU	3.2
1	A	363	LEU	3.2
2	B	129	PHE	3.2
2	B	171	VAL	3.2
1	A	335	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	266	ARG	3.1
2	B	113	LEU	3.1
1	A	286	ASP	3.1
2	B	180	TYR	3.1
2	B	163	ILE	3.1
1	A	142	ARG	3.1
2	B	124	THR	3.1
2	B	104	CYS	3.1
1	A	60	SER	3.0
2	B	121	ILE	3.0
1	A	348	LYS	3.0
1	A	89	GLN	3.0
2	B	417	GLN	3.0
2	B	377	GLY	3.0
2	B	115	ASP	3.0
1	A	260	VAL	3.0
1	A	324	GLU	2.9
1	A	86	PRO	2.9
1	A	307	SER	2.9
2	B	43	VAL	2.9
2	B	394	LEU	2.9
2	B	199	VAL	2.9
1	A	302	LEU	2.9
1	A	333	ILE	2.8
2	B	210	VAL	2.8
2	B	181	LEU	2.8
1	A	277	TRP	2.8
1	A	293	PRO	2.8
2	B	28	PRO	2.8
1	A	195	GLN	2.8
2	B	32	ARG	2.8
2	B	99	SER	2.8
2	B	118	ILE	2.8
1	A	264	LEU	2.8
1	A	268	LYS	2.8
1	A	271	PRO	2.8
1	A	224	ASP	2.8
1	A	322	MET	2.8
2	B	381	MET	2.7
1	A	327	CYS	2.7
2	B	139	GLY	2.7
2	B	125	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	72	TRP	2.7
2	B	225	THR	2.7
2	B	111	LEU	2.7
1	A	242	PHE	2.7
1	A	305	SER	2.6
2	B	36	GLN	2.6
2	B	126	VAL	2.6
2	B	392	ASN	2.6
2	B	383	HIS	2.6
1	A	346	LYS	2.6
1	A	178	TRP	2.6
1	A	218	ASN	2.6
1	A	276	ALA	2.5
1	A	265	GLU	2.5
2	B	166	GLU	2.5
2	B	170	ASN	2.5
2	B	194	HIS	2.5
1	A	329	ASN	2.5
2	B	35	LEU	2.5
1	A	190	ALA	2.4
2	B	240	GLY	2.4
2	B	168	ALA	2.4
1	A	95	LYS	2.4
1	A	310	TYR	2.4
2	B	62	TYR	2.4
1	A	269	LEU	2.4
1	A	201	HIS	2.4
2	B	418	LYS	2.4
2	B	95	CYS	2.4
1	A	211	GLN	2.4
1	A	88	VAL	2.4
1	A	236	VAL	2.4
1	A	330	LYS	2.3
2	B	37	ASP	2.3
2	B	42	THR	2.3
2	B	176	LYS	2.3
1	A	84	PRO	2.3
1	A	97	ARG	2.3
1	A	272	HIS	2.3
1	A	287	ARG	2.3
1	A	228	LYS	2.3
2	B	108	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	68	ASP	2.3
2	B	82	LEU	2.2
1	A	237	TRP	2.2
1	A	362	SER	2.2
1	A	158	ILE	2.2
1	A	220	LEU	2.2
1	A	256	LEU	2.2
2	B	214	THR	2.2
2	B	319	GLY	2.2
1	A	318	ILE	2.2
2	B	311	LEU	2.2
2	B	223	GLU	2.2
2	B	333	GLN	2.2
2	B	380	ALA	2.1
2	B	160	LEU	2.1
2	B	156	ALA	2.1
2	B	217	ILE	2.1
2	B	313	ARG	2.1
1	A	187	GLU	2.1
2	B	411	ALA	2.1
1	A	125	GLU	2.1
1	A	166	TYR	2.1
1	A	223	VAL	2.1
2	B	169	TYR	2.1
1	A	230	ASP	2.1
1	A	219	GLU	2.1
2	B	413	THR	2.1
1	A	144	LEU	2.1
1	A	121	ARG	2.1
2	B	85	GLY	2.1
2	B	284	PHE	2.1
2	B	172	ILE	2.0
2	B	178	LEU	2.0
2	B	157	VAL	2.0
1	A	109	ARG	2.0
2	B	177	LEU	2.0
1	A	252	ASP	2.0
1	A	209	VAL	2.0
2	B	183	SER	2.0
2	B	373	ALA	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)

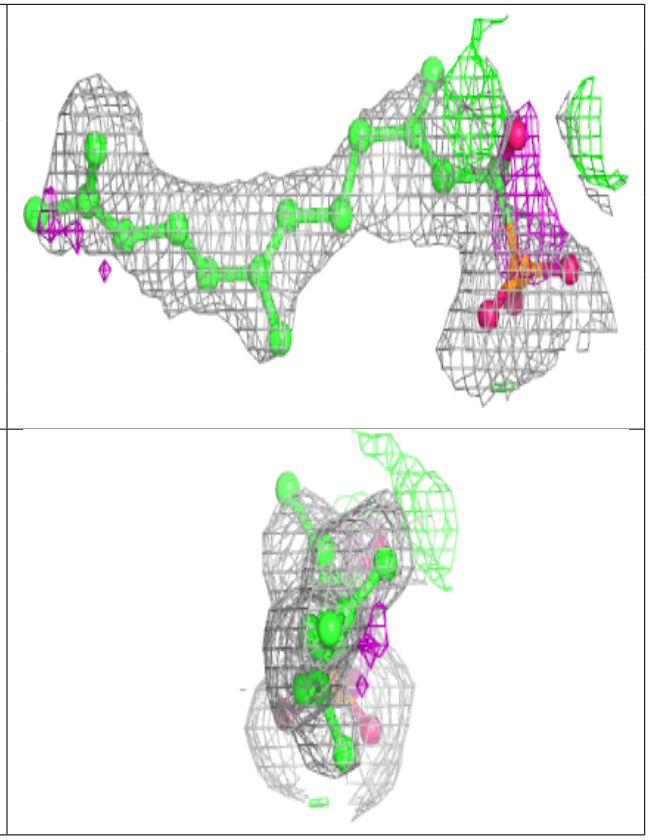
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

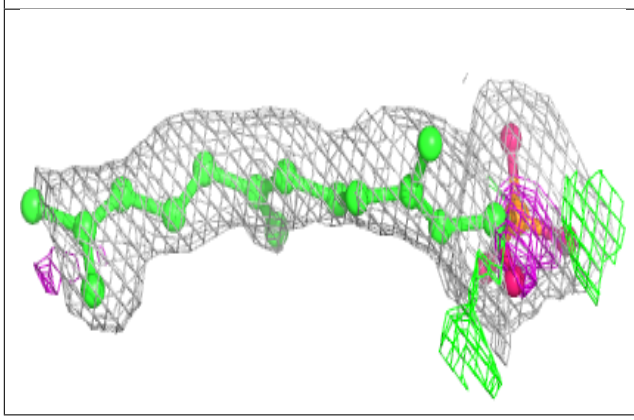
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HFP	B	501	20/20	0.76	0.31	30,30,30,30	0
5	FTH	B	1001	38/38	0.82	0.28	30,30,30,30	0
3	ZN	B	500	1/1	0.98	0.17	30,30,30,30	0

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 HFP B 501:

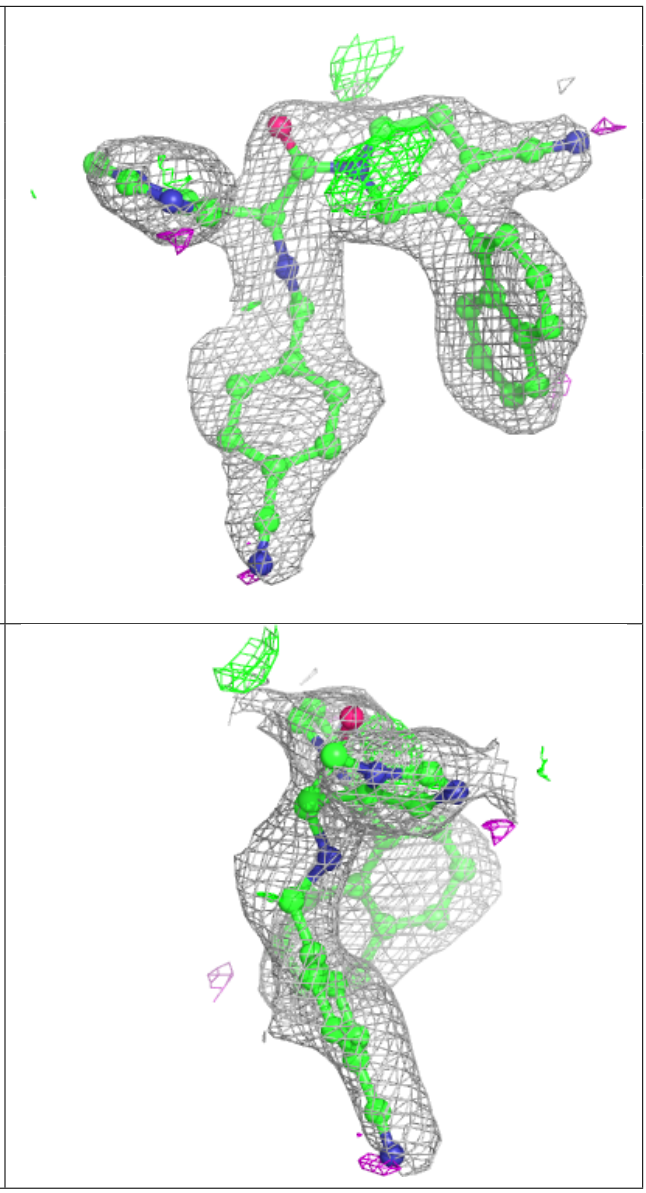
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around FTH B 1001:

$2mF_o$-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.