



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:28 pm BST

PDB ID : 1QBQ
Title : STRUCTURE OF RAT FARNESYL PROTEIN TRANSFERASE COM-
PLEXED WITH A CVIM PEPTIDE AND ALPHA-HYDROXYFARNE
SYLPHOSPHONIC ACID.
Authors : Strickland, C.L.; Windsor, W.T.; Syto, R.; Wang, L.; Bond, R.; Wu, Z.;
Schwartz, J.; Le, H.V.; Beese, L.S.; Weber, P.C.
Deposited on : 1999-04-27
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

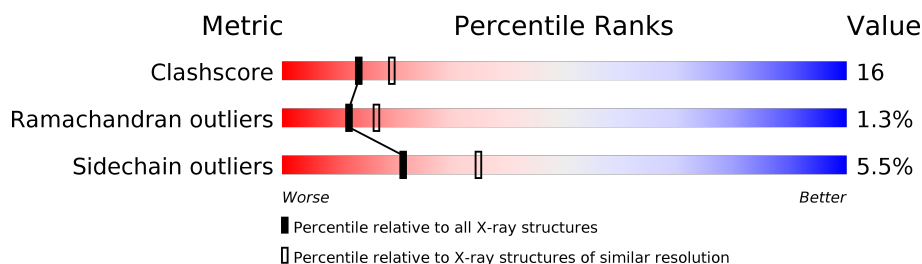
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	333	
2	B	437	
3	P	5	

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	ACT	A	2002	-	-	X	-
6	HFP	B	2001	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6154 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 FPT ALPHA-SUBUNIT.

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

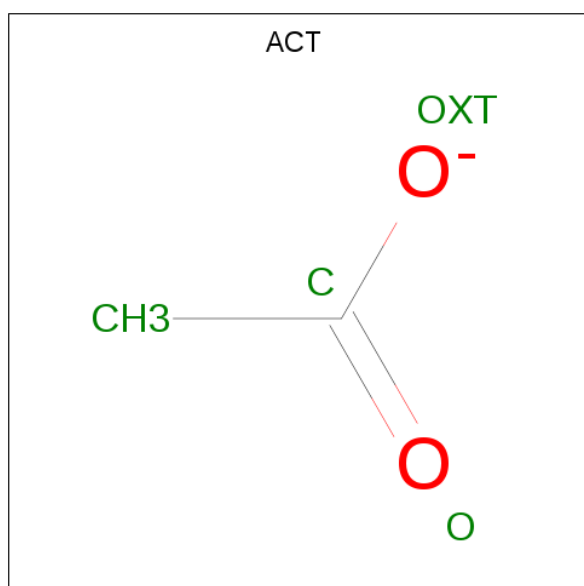
- Molecule 2 is a protein called FPT BETA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3153	2016	543	571	23			

- Molecule 3 is a protein called ACETYL-CYS-VAL-ILE-SELENOMET-COOH PEPTIDE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	P	5	Total	C	N	O	S	Se	0	0	0
			33	21	4	6	1	1			

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

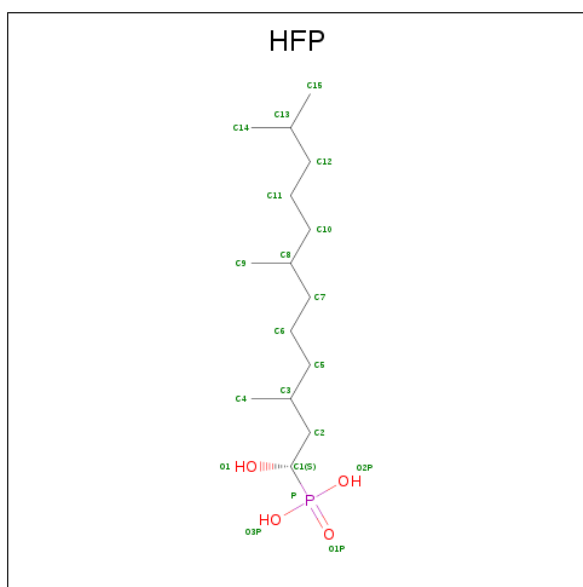


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is ALPHA-HYDROXYFARNESYLPHOSPHONIC ACID (three-letter code: HFP) (formula: C₁₅H₃₃O₄P).



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

- Molecule 7 is water.

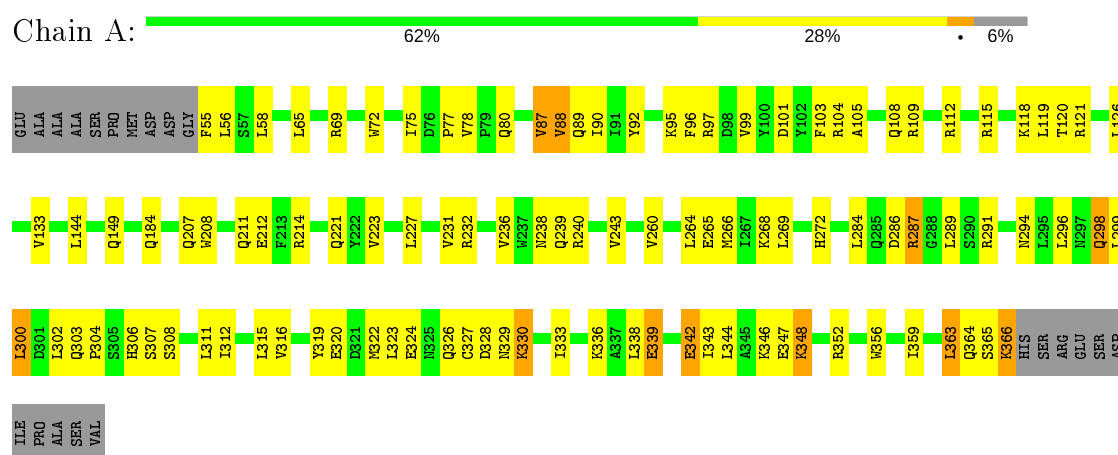
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	137	Total	O	0	0
			137	137		
7	B	139	Total	O	0	0
			139	139		
7	P	8	Total	O	0	0
			8	8		

3 Residue-property plots

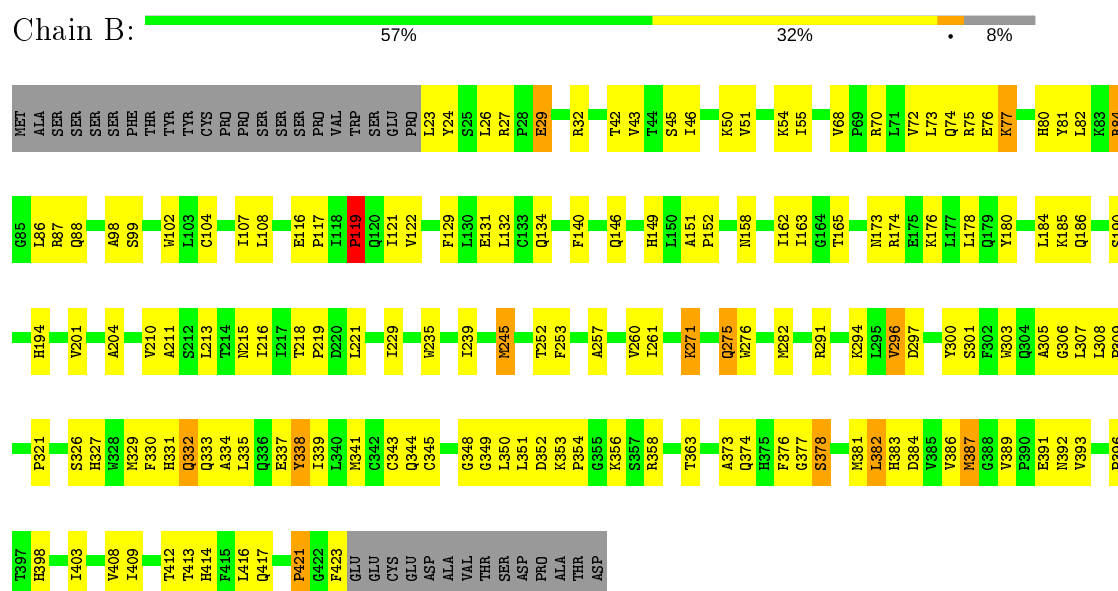
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: FPT ALPHA-SUBUNIT



• Molecule 2: FPT BETA-SUBUNIT



• Molecule 3: ACETYL-CYS-VAL-ILE-SELENOMET-COOH PEPTIDE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	174.13Å 174.13Å 69.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.218 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6154	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

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, ACE, ACT

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	0.54	0/2725	0.72	0/3700
2	B	0.56	0/3238	0.75	0/4397
3	P	1.35	0/29	0.82	0/35
All	All	0.56	0/5992	0.74	0/8132

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

There are no bond length outliers.

There are no bond angle outliers.

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	73	0
2	B	3153	0	3085	112	0
3	P	33	0	36	2	0
4	A	3	0	0	3	0
5	B	1	0	0	0	0
6	B	20	0	28	2	0
7	A	137	0	0	1	0
7	B	139	0	0	5	0
7	P	8	0	0	0	0
All	All	6154	0	5734	186	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 16.

All (186) 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:HE2	2:B:245:MET:HA	1.56	0.87
2:B:271:LYS:HE3	2:B:271:LYS:HA	1.58	0.85
2:B:77:LYS:HA	2:B:77:LYS:HE3	1.57	0.85
2:B:338:TYR:CE2	2:B:343:CYS:SG	2.71	0.83
1:A:322:MET:HE3	1:A:333:ILE:HD13	1.63	0.79
2:B:178:LEU:HD12	2:B:421:PRO:HB2	1.64	0.77
1:A:312:ILE:O	1:A:316:VAL:HG23	1.85	0.77
2:B:185:LYS:HE3	2:B:221:LEU:O	1.85	0.76
2:B:218:THR:HB	2:B:219:PRO:HD2	1.68	0.74
2:B:178:LEU:HG	2:B:216:ILE:HB	1.71	0.73
2:B:84:ARG:HH22	2:B:88:GLN:HG2	1.54	0.71
4:A:2002:ACT:OXT	4:A:2002:ACT:CH3	2.40	0.69
7:A:1132:HOH:O	2:B:43:VAL:HG23	1.91	0.69
1:A:312:ILE:HD12	1:A:348:LYS:HG2	1.76	0.68
1:A:327:CYS:O	1:A:330:LYS:HB3	1.94	0.68
1:A:287:ARG:HD3	1:A:291:ARG:HD3	1.76	0.67
4:A:2002:ACT:O	4:A:2002:ACT:CH3	2.42	0.67
2:B:82:LEU:HD21	2:B:363:THR:HG21	1.77	0.66
2:B:73:LEU:HD12	2:B:344:GLN:OE1	1.96	0.65
1:A:344:LEU:HD23	1:A:348:LYS:HB3	1.78	0.65
1:A:365:SER:HB2	1:A:366:LYS:HD3	1.78	0.64
6:B:2001:HFP:H92	3:P:3:ILE:HG22	1.80	0.64
2:B:335:LEU:O	2:B:339:ILE:HG13	1.98	0.64
2:B:253:PHE:HA	2:B:307:LEU:HD21	1.80	0.64
1:A:359:ILE:O	1:A:363:LEU:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:HIS:HB3	2:B:332:GLN:HE22	1.64	0.63
1:A:343:ILE:HG22	1:A:348:LYS:HB2	1.80	0.63
2:B:72:VAL:HG22	2:B:389:VAL:HG21	1.81	0.63
2:B:116:GLU:HB3	2:B:117:PRO:HD2	1.80	0.63
2:B:73:LEU:O	2:B:75:ARG:N	2.33	0.62
1:A:80:GLN:HB2	1:A:104:ARG:CZ	2.29	0.62
1:A:347:GLU:HG2	1:A:348:LYS:HE3	1.81	0.62
2:B:51:VAL:HA	2:B:54:LYS:HE2	1.82	0.61
1:A:268:LYS:HE2	1:A:302:LEU:HD11	1.82	0.61
1:A:302:LEU:HD22	1:A:306:HIS:CD2	2.35	0.61
1:A:223:VAL:HG11	1:A:240:ARG:HB2	1.82	0.60
2:B:301:SER:O	2:B:305:ALA:HB3	2.01	0.59
2:B:398:HIS:CD2	2:B:408:VAL:HG11	2.37	0.59
2:B:73:LEU:H	2:B:392:ASN:ND2	2.01	0.59
2:B:84:ARG:NH2	2:B:88:GLN:HG2	2.17	0.59
2:B:239:ILE:HB	2:B:252:THR:HA	1.84	0.59
2:B:98:ALA:HA	2:B:146:GLN:HE22	1.67	0.58
2:B:151:ALA:HB3	2:B:152:PRO:HD3	1.84	0.58
4:A:2002:ACT:O	4:A:2002:ACT:OXT	2.22	0.58
2:B:353:LYS:HB2	2:B:354:PRO:HD2	1.85	0.57
2:B:337:GLU:HB3	2:B:341:MET:HE3	1.86	0.57
2:B:194:HIS:HB2	7:B:1238:HOH:O	2.05	0.56
1:A:149:GLN:HE22	1:A:184:GLN:HE22	1.53	0.55
1:A:55:PHE:HB2	1:A:118:LYS:HD3	1.88	0.55
1:A:90:ILE:HB	1:A:92:TYR:CE2	2.40	0.55
2:B:308:LEU:HD13	2:B:330:PHE:HB3	1.88	0.55
2:B:398:HIS:CD2	2:B:408:VAL:HG21	2.42	0.55
1:A:104:ARG:O	1:A:108:GLN:HB2	2.06	0.55
2:B:257:ALA:O	2:B:261:ILE:HG13	2.07	0.55
2:B:180:TYR:CZ	2:B:184:LEU:HD11	2.42	0.54
1:A:303:GLN:O	1:A:307:SER:HB2	2.07	0.54
2:B:386:VAL:HG21	2:B:393:VAL:HB	1.88	0.54
1:A:208:TRP:NE1	1:A:212:GLU:HG3	2.22	0.54
1:A:319:TYR:HD2	1:A:322:MET:HE2	1.72	0.54
1:A:72:TRP:CE3	1:A:75:ILE:HD12	2.43	0.53
2:B:352:ASP:HB3	2:B:356:LYS:HG3	1.90	0.53
1:A:366:LYS:N	1:A:366:LYS:HD3	2.23	0.53
2:B:412:THR:O	2:B:416:LEU:HB2	2.08	0.53
1:A:342:GLU:OE1	1:A:346:LYS:HE3	2.09	0.53
1:A:286:ASP:O	1:A:287:ARG:HB2	2.09	0.53
2:B:158:ASN:O	2:B:162:ILE:HG13	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:VAL:HG23	1:A:105:ALA:HB2	1.91	0.52
1:A:294:ASN:O	1:A:298:GLN:HG2	2.09	0.52
2:B:186:GLN:HB2	2:B:190:SER:O	2.10	0.52
2:B:23:LEU:O	2:B:27:ARG:HG3	2.09	0.52
1:A:287:ARG:HD3	1:A:287:ARG:O	2.08	0.52
2:B:104:CYS:O	2:B:108:LEU:HB2	2.09	0.52
2:B:308:LEU:CD1	2:B:330:PHE:HB3	2.40	0.52
1:A:338:LEU:HD11	1:A:364:GLN:HE22	1.75	0.52
2:B:374:GLN:O	2:B:384:ASP:HA	2.10	0.52
2:B:282:MET:CG	2:B:296:VAL:HG13	2.40	0.51
2:B:348:GLY:O	2:B:358:ARG:HD2	2.10	0.51
2:B:134:GLN:HB2	2:B:140:PHE:CE2	2.46	0.51
2:B:75:ARG:NH2	2:B:391:GLU:O	2.43	0.51
1:A:356:TRP:HA	1:A:356:TRP:CE3	2.44	0.51
1:A:296:LEU:O	1:A:300:LEU:HB2	2.12	0.50
1:A:312:ILE:CD1	1:A:348:LYS:HG2	2.41	0.50
1:A:80:GLN:HB2	1:A:104:ARG:NH2	2.27	0.50
2:B:86:LEU:HB2	2:B:107:ILE:HG21	1.93	0.50
2:B:326:SER:O	2:B:383:HIS:HB3	2.11	0.50
2:B:282:MET:HG3	2:B:296:VAL:HG13	1.94	0.50
2:B:72:VAL:HG22	2:B:389:VAL:CG2	2.39	0.50
2:B:381:MET:O	2:B:382:LEU:HD22	2.12	0.50
2:B:245:MET:CE	2:B:245:MET:HA	2.37	0.50
2:B:398:HIS:HD2	2:B:408:VAL:HG11	1.77	0.50
2:B:76:GLU:O	2:B:80:HIS:ND1	2.45	0.50
2:B:46:ILE:HG22	2:B:50:LYS:HE3	1.94	0.49
2:B:297:ASP:HB3	2:B:300:TYR:HD1	1.77	0.49
2:B:50:LYS:O	2:B:54:LYS:HG3	2.13	0.49
1:A:312:ILE:HG22	1:A:344:LEU:HD11	1.94	0.48
2:B:216:ILE:HG22	2:B:421:PRO:CD	2.43	0.48
2:B:119:PRO:O	2:B:122:VAL:HG12	2.13	0.48
2:B:55:ILE:HD13	2:B:354:PRO:HG3	1.95	0.48
2:B:121:ILE:N	2:B:121:ILE:HD12	2.28	0.48
1:A:302:LEU:HD22	1:A:306:HIS:HD2	1.77	0.48
2:B:326:SER:HB2	2:B:383:HIS:CD2	2.49	0.48
1:A:75:ILE:HD11	1:A:115:ARG:CZ	2.44	0.48
1:A:223:VAL:HG13	1:A:236:VAL:HG12	1.95	0.47
1:A:238:ASN:HA	2:B:235:TRP:CZ2	2.49	0.47
2:B:389:VAL:HG12	2:B:391:GLU:HB2	1.96	0.47
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.49	0.47
1:A:77:PRO:HB2	1:A:101:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PHE:HA	1:A:126:LEU:HD13	1.96	0.47
2:B:376:PHE:CZ	2:B:378:SER:HB2	2.50	0.47
2:B:344:GLN:HA	2:B:350:LEU:HD13	1.96	0.46
1:A:239:GLN:O	1:A:243:VAL:HG23	2.15	0.46
1:A:58:LEU:O	1:A:95:LYS:NZ	2.45	0.46
1:A:72:TRP:CZ3	1:A:75:ILE:HD12	2.51	0.46
1:A:92:TYR:HB2	1:A:97:ARG:HG3	1.97	0.46
2:B:403:ILE:HG13	2:B:408:VAL:HG23	1.98	0.46
2:B:121:ILE:HD12	2:B:121:ILE:H	1.81	0.46
2:B:414:HIS:O	2:B:417:GLN:HG2	2.16	0.46
2:B:23:LEU:HD12	2:B:26:LEU:CD1	2.45	0.46
1:A:99:VAL:HG13	1:A:119:LEU:CD1	2.46	0.46
1:A:316:VAL:O	1:A:320:GLU:HG3	2.16	0.46
2:B:46:ILE:O	2:B:50:LYS:HG3	2.16	0.45
2:B:149:HIS:HB3	2:B:152:PRO:HD2	1.98	0.45
2:B:303:TRP:CH2	6:B:2001:HFP:H121	2.52	0.45
2:B:131:GLU:HG3	7:B:1129:HOH:O	2.16	0.45
1:A:89:GLN:OE1	2:B:87:ARG:NH2	2.49	0.45
1:A:65:LEU:O	1:A:69:ARG:HG3	2.16	0.45
1:A:87:VAL:O	1:A:88:VAL:C	2.55	0.45
2:B:275:GLN:HE21	2:B:276:TRP:N	2.13	0.45
2:B:308:LEU:HD22	2:B:329:MET:HB2	1.99	0.45
1:A:338:LEU:HD21	1:A:363:LEU:HB3	1.99	0.44
1:A:339:GLU:O	1:A:343:ILE:HG13	2.18	0.44
1:A:319:TYR:CE1	1:A:336:LYS:HG3	2.53	0.44
1:A:72:TRP:CZ2	1:A:115:ARG:HD2	2.52	0.44
1:A:103:PHE:HE1	1:A:120:THR:HG22	1.83	0.43
2:B:335:LEU:HD23	2:B:373:ALA:HB2	2.00	0.43
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.93	0.43
2:B:129:PHE:O	2:B:132:LEU:HB2	2.19	0.43
1:A:260:VAL:HG21	1:A:284:LEU:HD21	2.00	0.43
2:B:108:LEU:O	2:B:162:ILE:HG21	2.19	0.43
2:B:333:GLN:HG3	2:B:387:MET:CE	2.48	0.43
2:B:73:LEU:H	2:B:392:ASN:HD21	1.65	0.43
2:B:99:SER:O	2:B:102:TRP:HB2	2.18	0.43
1:A:328:ASP:O	1:A:329:ASN:HB2	2.19	0.43
2:B:378:SER:HB3	2:B:381:MET:HG3	2.00	0.43
2:B:24:TYR:HB2	2:B:333:GLN:CD	2.40	0.43
2:B:81:TYR:CE2	2:B:349:GLY:HA3	2.54	0.43
1:A:105:ALA:O	1:A:109:ARG:HG3	2.18	0.42
1:A:311:LEU:O	1:A:315:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HG	1:A:236:VAL:CG1	2.48	0.42
1:A:207:GLN:O	1:A:211:GLN:HB2	2.20	0.42
2:B:51:VAL:O	2:B:55:ILE:HG12	2.19	0.42
2:B:331:HIS:CD2	2:B:334:ALA:H	2.38	0.42
2:B:409:ILE:O	2:B:413:THR:HG23	2.20	0.42
2:B:291:ARG:HB2	2:B:294:LYS:HG3	2.01	0.42
1:A:272:HIS:CD2	1:A:308:SER:HB3	2.55	0.41
2:B:291:ARG:HB2	2:B:294:LYS:CG	2.50	0.41
1:A:287:ARG:CD	1:A:291:ARG:HD3	2.49	0.41
1:A:363:LEU:HA	1:A:363:LEU:HD12	1.89	0.41
2:B:152:PRO:HG3	3:P:4:MSE:HE1	2.02	0.41
2:B:210:VAL:HG23	2:B:211:ALA:N	2.35	0.41
2:B:260:VAL:HG22	7:B:1270:HOH:O	2.20	0.41
2:B:330:PHE:HA	7:B:1188:HOH:O	2.20	0.41
1:A:302:LEU:HB3	1:A:306:HIS:HB2	2.03	0.41
1:A:320:GLU:O	1:A:324:GLU:HG3	2.21	0.41
2:B:211:ALA:HA	2:B:216:ILE:HD11	2.02	0.41
2:B:338:TYR:HE2	2:B:343:CYS:SG	2.34	0.41
2:B:204:ALA:HB1	2:B:229:ILE:HD11	2.01	0.41
2:B:213:LEU:HD23	2:B:412:THR:HG22	2.03	0.41
2:B:211:ALA:HA	2:B:216:ILE:CG1	2.51	0.41
2:B:306:GLY:O	2:B:309:PRO:HD2	2.21	0.41
2:B:163:ILE:HG22	2:B:165:THR:HG23	2.02	0.41
2:B:173:ASN:CG	2:B:176:LYS:HB2	2.41	0.41
1:A:112:ARG:O	1:A:144:LEU:HD21	2.21	0.41
2:B:29:GLU:O	2:B:32:ARG:HD2	2.20	0.41
2:B:350:LEU:HB2	2:B:363:THR:HA	2.02	0.40
2:B:396:PRO:HD2	7:B:1271:HOH:O	2.21	0.40
1:A:232:ARG:NH1	2:B:42:THR:HG23	2.35	0.40
1:A:299:LEU:O	1:A:311:LEU:HD11	2.22	0.40
2:B:216:ILE:HG22	2:B:421:PRO:HD2	2.03	0.40
2:B:345:CYS:HB3	2:B:349:GLY:O	2.22	0.40
1:A:231:VAL:HG21	1:A:266:MET:HE2	2.02	0.40
1:A:58:LEU:HD22	1:A:95:LYS:HE3	2.03	0.40
2:B:376:PHE:CG	2:B:377:GLY:N	2.89	0.40
1:A:231:VAL:HG21	1:A:266:MET:CE	2.51	0.40
2:B:174:ARG:NH2	2:B:215:ASN:O	2.53	0.40
2:B:24:TYR:HB2	2:B:333:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	310/333 (93%)	282 (91%)	24 (8%)	4 (1%)	12	17
2	B	399/437 (91%)	371 (93%)	23 (6%)	5 (1%)	12	17
3	P	3/5 (60%)	3 (100%)	0	0	100	100
All	All	712/775 (92%)	656 (92%)	47 (7%)	9 (1%)	12	17

All (9) 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	304	PRO
2	B	421	PRO
1	A	88	VAL
2	B	119	PRO
2	B	321	PRO

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	291/307 (95%)	273 (94%)	18 (6%)	18	29
2	B	338/371 (91%)	321 (95%)	17 (5%)	24	40
3	P	4/3 (133%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	633/681 (93%)	598 (94%)	35 (6%)	21	35

All (35) 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	214	ARG
1	A	221	GLN
1	A	265	GLU
1	A	269	LEU
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	119	PRO
2	B	201	VAL
2	B	245	MET
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	149	GLN
1	A	184	GLN
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
2	B	398	HIS
2	B	410	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
6	HFP	B	2001	-	17,19,19	1.75	5 (29%)	22,25,25	2.27	7 (31%)

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
6	HFP	B	2001	-	2/2/5/5	8/22/22/22	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2001	HFP	C2-C3	-4.63	1.34	1.53
6	B	2001	HFP	C7-C8	-3.33	1.35	1.52
6	B	2001	HFP	O1-C1	2.43	1.44	1.41
6	B	2001	HFP	P-O1P	-2.33	1.45	1.49
6	B	2001	HFP	C12-C13	-2.27	1.36	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2001	HFP	C3-C2-C1	7.52	122.84	115.21
6	B	2001	HFP	C4-C3-C2	3.02	120.51	110.89
6	B	2001	HFP	C2-C3-C5	2.55	120.43	111.98
6	B	2001	HFP	C9-C8-C7	2.42	120.05	111.29
6	B	2001	HFP	C4-C3-C5	2.15	119.06	111.29
6	B	2001	HFP	O1P-P-C1	-2.08	107.89	112.94
6	B	2001	HFP	C9-C8-C10	2.04	118.67	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	2001	HFP	C3
6	B	2001	HFP	C8

All (8) torsion outliers are listed below:

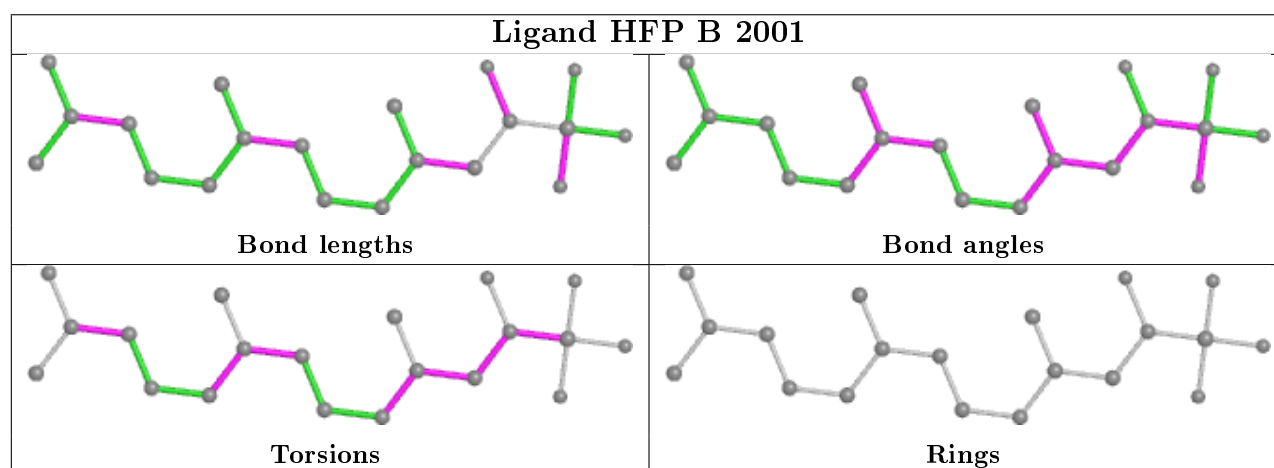
Mol	Chain	Res	Type	Atoms
6	B	2001	HFP	P-C1-C2-C3
6	B	2001	HFP	C1-C2-C3-C4
6	B	2001	HFP	C6-C7-C8-C9
6	B	2001	HFP	C11-C12-C13-C14
6	B	2001	HFP	C4-C3-C5-C6
6	B	2001	HFP	O1-C1-C2-C3
6	B	2001	HFP	C2-C1-P-O1P
6	B	2001	HFP	C11-C10-C8-C9

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2001	HFP	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.