



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:19 AM UTC

PDB ID : 1QBQ / pdb_00001qbq
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 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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

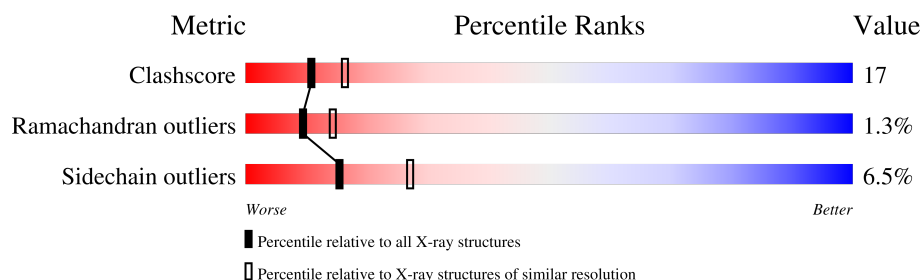
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	333	58% 31% 5% 6%
2	B	437	52% 34% 5% 8%
3	P	5	60% 20% 20%

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			

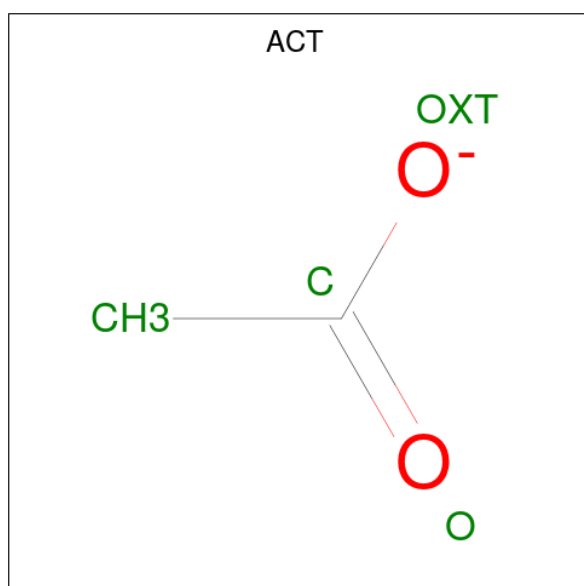
- Molecule 2 is a protein called FPT BETA-SUBUNIT.

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 (CCD ID: ACT) (formula: C₂H₃O₂).

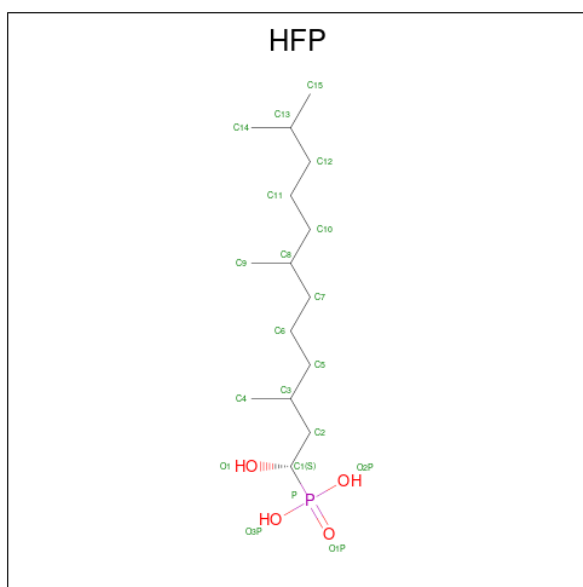


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is ALPHA-HYDROXYFARNESYLPHOSPHONIC ACID (CCD ID: 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.

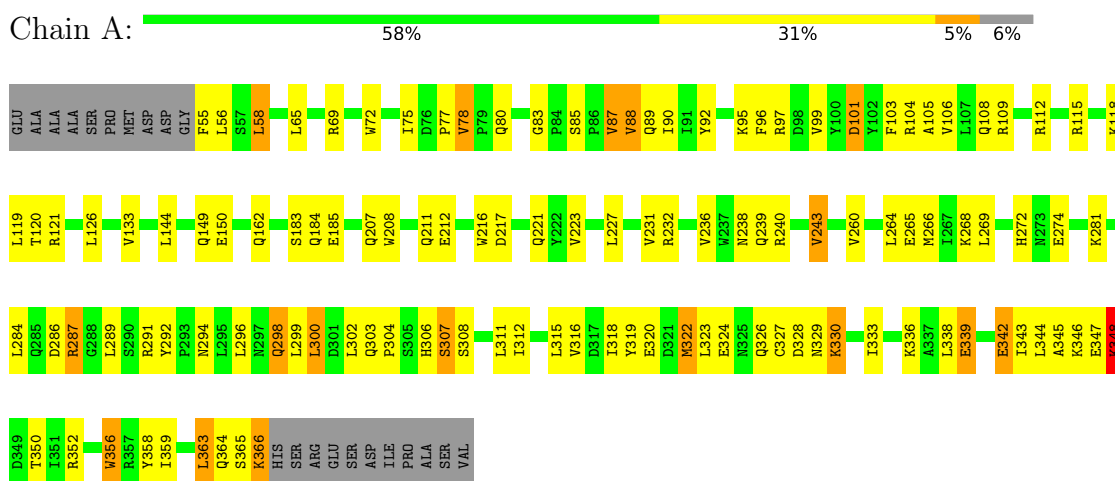
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	137	Total	O	0	0
			137	137		
7	B	139	Total	O	0	0
			139	139		
7	P	8	Total	O	0	0
			8	8		

3 Residue-property plots

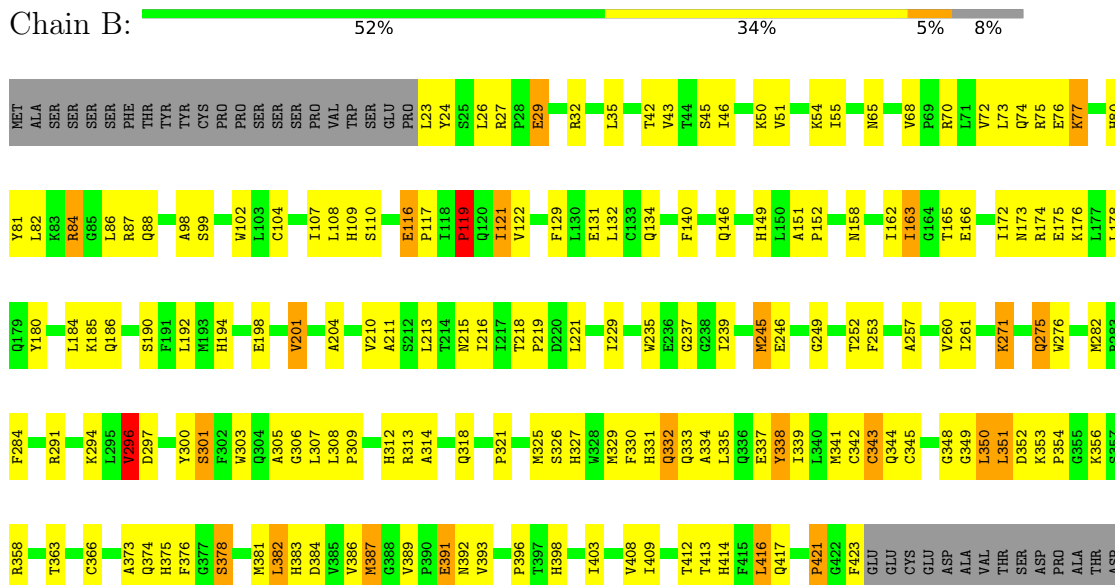
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

Chain P: 60% 20% 20%



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, ACT, ZN, ACE

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	0.66	0/2725	1.13	24/3700 (0.6%)
2	B	0.68	0/3238	1.17	23/4397 (0.5%)
3	P	1.92	2/29 (6.9%)	0.93	0/35
All	All	0.68	2/5992 (0.0%)	1.15	47/8132 (0.6%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	4	MSE	SE-CE	-5.90	1.77	1.95
3	P	4	MSE	CG-SE	-5.20	1.79	1.95

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	LYS	N-CA-C	10.10	123.32	111.71
1	A	185	GLU	N-CA-C	9.63	122.77	111.02
2	B	342	CYS	N-CA-C	8.06	123.46	112.90
2	B	163	ILE	N-CA-C	-7.75	103.14	110.42
2	B	116	GLU	CA-C-N	7.58	128.18	120.14
2	B	116	GLU	C-N-CA	7.58	128.18	120.14
2	B	296	VAL	CB-CA-C	-7.49	103.06	111.45
1	A	217	ASP	N-CA-C	6.97	122.87	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLU	N-CA-C	6.85	118.74	111.28
1	A	216	TRP	N-CA-C	6.84	120.85	112.23
2	B	301	SER	N-CA-C	-6.59	104.17	111.82
1	A	78	VAL	CA-C-N	6.37	126.55	120.31
1	A	78	VAL	C-N-CA	6.37	126.55	120.31
2	B	366	CYS	N-CA-C	-6.35	104.44	111.36
2	B	312	HIS	N-CA-C	-6.29	103.12	111.24
2	B	237	GLY	N-CA-C	-6.27	107.23	114.69
1	A	150	GLU	N-CA-C	-6.27	104.53	111.36
1	A	292	TYR	CA-C-N	6.24	125.45	118.97
1	A	292	TYR	C-N-CA	6.24	125.45	118.97
1	A	101	ASP	N-CA-C	-5.90	104.85	111.28
2	B	201	VAL	N-CA-C	5.83	119.22	111.17
2	B	35	LEU	N-CA-C	5.71	118.60	110.10
2	B	110	SER	N-CA-C	-5.67	105.18	111.36
1	A	183	SER	N-CA-C	5.66	119.29	112.38
1	A	85	SER	CA-C-N	5.65	125.55	119.85
1	A	85	SER	C-N-CA	5.65	125.55	119.85
2	B	65	ASN	N-CA-C	5.64	120.16	113.28
1	A	307	SER	N-CA-C	5.64	119.43	109.96
2	B	192	LEU	N-CA-C	-5.56	102.29	110.52
2	B	351	LEU	N-CA-C	5.56	117.25	108.96
1	A	83	GLY	CA-C-N	5.55	126.78	119.84
1	A	83	GLY	C-N-CA	5.55	126.78	119.84
2	B	375	HIS	N-CA-C	5.52	117.41	108.41
2	B	172	ILE	N-CA-C	5.48	115.46	108.12
2	B	109	HIS	N-CA-C	-5.46	107.17	113.88
2	B	391	GLU	N-CA-C	-5.42	106.64	113.20
1	A	356	TRP	N-CA-C	5.32	117.83	111.71
1	A	350	THR	N-CA-C	5.30	119.37	113.01
2	B	249	GLY	N-CA-C	5.29	119.08	112.73
1	A	322	MET	N-CA-C	-5.28	106.79	113.18
2	B	343	CYS	N-CA-C	5.26	119.01	112.59
1	A	58	LEU	N-CA-C	-5.23	106.16	112.54
1	A	318	ILE	N-CA-C	-5.21	105.52	110.42
1	A	243	VAL	N-CA-C	5.20	115.35	110.30
2	B	198	GLU	N-CA-C	5.18	116.79	110.41
1	A	345	ALA	N-CA-C	5.08	116.90	111.36
2	B	318	GLN	N-CA-C	-5.05	107.62	112.97

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

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	74	0
2	B	3153	0	3085	118	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	192	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 17.

All (192) 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: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
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
2:B:245:MET:HE2	2:B:246:GLU:H	1.57	0.69
7:A:1132:HOH:O	2:B:43:VAL:HG23	1.91	0.69
1:A:322:MET:HE3	1:A:333:ILE:HD13	1.74	0.68
1:A:312:ILE:HD12	1:A:348:LYS:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TYR:HD2	1:A:322:MET:HE2	1.59	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:CH3	4:A:2002:ACT:O	2.42	0.67
2:B:82:LEU:HD21	2:B:363:THR:HG21	1.77	0.66
2:B:337:GLU:HB3	2:B:341:MET:HE3	1.78	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:325:MET:HE3	2:B:381:MET:SD	2.37	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
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:OXT	4:A:2002:ACT:O	2.22	0.58
2:B:353:LYS:HB2	2:B:354:PRO:HD2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ALA:O	2:B:261:ILE:HG13	2.07	0.55
2:B:245:MET:HA	2:B:245:MET:CE	2.37	0.54
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: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:HD3	1:A:366:LYS:N	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
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:23:LEU:O	2:B:27:ARG:HG3	2.09	0.52
2:B:186:GLN:HB2	2:B:190:SER:O	2.10	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:CE3	1:A:356:TRP:HA	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:72:VAL:HG22	2:B:389:VAL:CG2	2.39	0.50
2:B:282:MET:HG3	2:B:296:VAL:HG13	1.94	0.50
2:B:381:MET:O	2:B:382:LEU:HD22	2.12	0.50
2:B:76:GLU:O	2:B:80:HIS:ND1	2.45	0.50
2:B:398:HIS:HD2	2:B:408:VAL:HG11	1.77	0.50
1:A:87:VAL:O	1:A:88:VAL:C	2.55	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:55:ILE:HD13	2:B:354:PRO:HG3	1.95	0.48
2:B:119:PRO:O	2:B:122:VAL:HG12	2.13	0.48
2:B:121:ILE:HD12	2:B:121:ILE:N	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:77:PRO:HB2	1:A:101:ASP:HB3	1.96	0.47
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.49	0.47
2:B:24:TYR:HB2	2:B:333:GLN:CD	2.40	0.47
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:245:MET:HE2	2:B:245:MET:HA	1.97	0.46
2:B:344:GLN:HA	2:B:350:LEU:HD13	1.96	0.46
1:A:58:LEU:O	1:A:95:LYS:NZ	2.45	0.46
1:A:239:GLN:O	1:A:243:VAL:HG23	2.15	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:173:ASN:CG	2:B:176:LYS:HB2	2.41	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
2:B:23:LEU:HD13	2:B:341:MET:HE2	1.98	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:358:TYR:CD2	1:A:358:TYR:C	2.96	0.44
1:A:231:VAL:HG21	1:A:266:MET:HE2	1.98	0.44
1:A:338:LEU:HD21	1:A:363:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLU:O	1:A:343:ILE:HG13	2.18	0.44
1:A:72:TRP:CZ2	1:A:115:ARG:HD2	2.52	0.44
1:A:319:TYR:CE1	1:A:336:LYS:HG3	2.53	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
2:B:284:PHE:CD2	2:B:284:PHE:C	2.96	0.43
1:A:260:VAL:HG21	1:A:284:LEU:HD21	2.00	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
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
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: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
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:207:GLN:NE2	2:B:245:MET:HE3	2.35	0.41
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:HD12	1:A:363:LEU:HA	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:163:ILE:HG22	2:B:165:THR:HG23	2.02	0.41
2:B:211:ALA:HA	2:B:216:ILE:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:GLY:O	2:B:309:PRO:HD2	2.21	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:58:LEU:HD22	1:A:95:LYS:HE3	2.03	0.40
2:B:313:ARG:O	2:B:314:ALA:C	2.64	0.40
2:B:24:TYR:HB2	2:B:333:GLN:OE1	2.21	0.40
2:B:165:THR:O	2:B:166:GLU:C	2.64	0.40
2:B:174:ARG:NH2	2:B:215:ASN:O	2.53	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	310/333 (93%)	282 (91%)	24 (8%)	4 (1%)	9	14
2	B	399/437 (91%)	371 (93%)	23 (6%)	5 (1%)	9	14
3	P	3/5 (60%)	3 (100%)	0	0	100	100
All	All	712/775 (92%)	656 (92%)	47 (7%)	9 (1%)	9	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ARG
2	B	74	GLN
1	A	326	GLN

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Mol	Chain	Res	Type
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%)	271 (93%)	20 (7%)	14	24
2	B	338/371 (91%)	317 (94%)	21 (6%)	16	29
3	P	4/3 (133%)	4 (100%)	0	100	100
All	All	633/681 (93%)	592 (94%)	41 (6%)	15	27

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	87	VAL
1	A	106	VAL
1	A	121	ARG
1	A	162	GLN
1	A	221	GLN
1	A	265	GLU
1	A	269	LEU
1	A	281	LYS
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

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Mol	Chain	Res	Type
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	121	ILE
2	B	175	GLU
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	350	LEU
2	B	351	LEU
2	B	382	LEU
2	B	387	MET
2	B	416	LEU
2	B	423	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	108	GLN
1	A	135	HIS
1	A	149	GLN
1	A	204	GLN
1	A	221	GLN
1	A	278	ASN
1	A	294	ASN
1	A	306	HIS
1	A	325	ASN
1	A	364	GLN
2	B	48	GLN
2	B	146	GLN

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Mol	Chain	Res	Type
2	B	327	HIS
2	B	331	HIS
2	B	332	GLN
2	B	375	HIS
2	B	392	ASN
2	B	398	HIS
2	B	402	ASN
2	B	410	GLN

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 oligosaccharides 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	$\# Z > 2$
6	HFP	B	2001	-	16,19,19	1.80	4 (25%)	20,25,25	2.36	6 (30%)

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	9/22/22/22	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2001	HFP	C2-C3	-4.93	1.34	1.53
6	B	2001	HFP	C7-C8	-3.61	1.35	1.52
6	B	2001	HFP	C12-C13	-2.47	1.36	1.51
6	B	2001	HFP	P-O1P	-2.34	1.45	1.49

All (6) 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	3.16	120.51	110.84
6	B	2001	HFP	C2-C3-C5	2.62	120.43	111.86
6	B	2001	HFP	C9-C8-C7	2.46	120.05	111.27
6	B	2001	HFP	C4-C3-C5	2.18	119.06	111.27
6	B	2001	HFP	C9-C8-C10	2.07	118.67	111.27

All (2) chirality outliers are listed below:

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

All (9) torsion outliers are listed below:

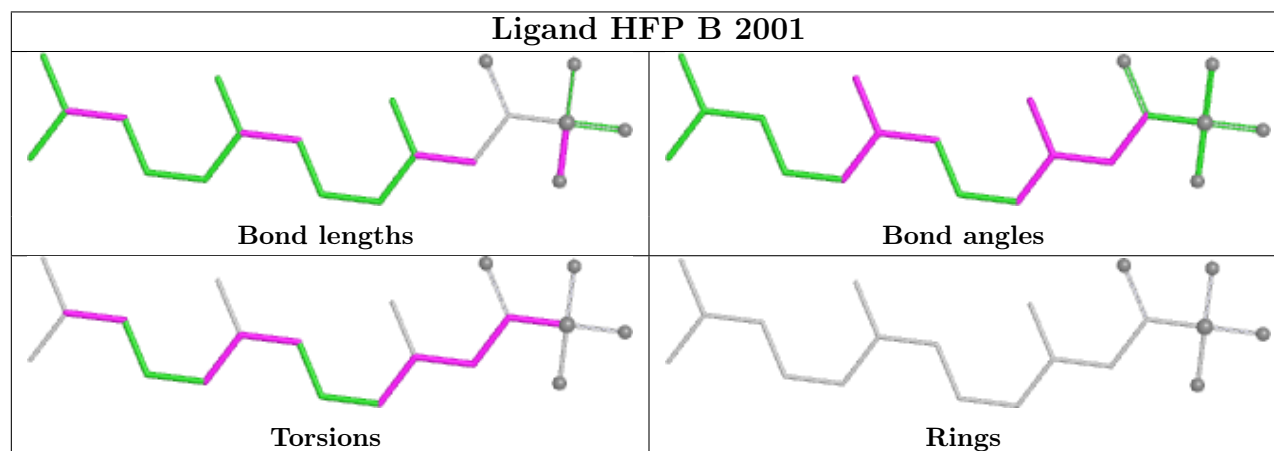
Mol	Chain	Res	Type	Atoms
6	B	2001	HFP	O1-C1-P-O1P
6	B	2001	HFP	P-C1-C2-C3
6	B	2001	HFP	C1-C2-C3-C4
6	B	2001	HFP	C6-C7-C8-C9
6	B	2001	HFP	C11-C12-C13-C14
6	B	2001	HFP	O1-C1-C2-C3
6	B	2001	HFP	C2-C1-P-O1P
6	B	2001	HFP	C11-C10-C8-C9
6	B	2001	HFP	C4-C3-C5-C6

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 [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

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.