



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:34 AM UTC

PDB ID : 1RTI / pdb_00001rti
Title : HIGH RESOLUTION STRUCTURES OF HIV-1 RT FROM FOUR RT-INHIBITOR COMPLEXES
Authors : Ren, J.; Esnouf, R.; Garman, E.; Somers, D.; Ross, C.; Kirby, I.; Keeling, J.; Darby, G.; Jones, Y.; Stuart, D.; Stammers, D.
Deposited on : 1995-05-03
Resolution : 3.00 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)	:	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

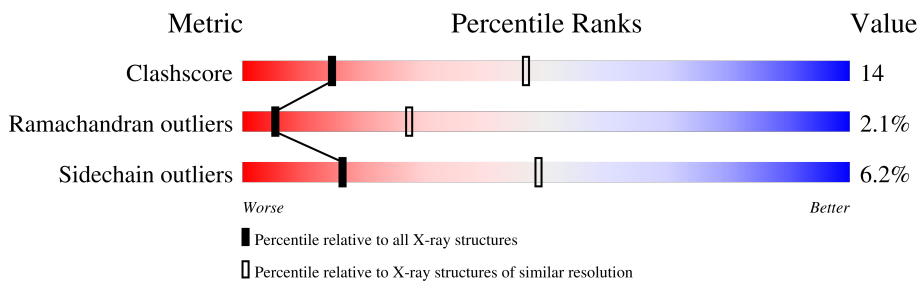
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	560	 64% 29% . . .
2	B	440	 60% 29% . 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7857 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.

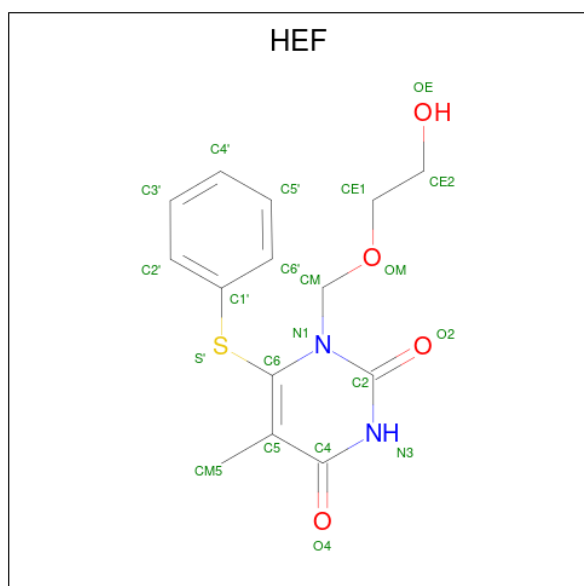
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4435	2869	739	819	8			

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	413	Total	C	N	O	S	0	0	0
			3401	2210	565	619	7			

- Molecule 3 is 1-(2-HYDROXYETHYLOXYMETHYL)-6-PHENYL THIOTHYMININE (CCD ID: HEF) (formula: $C_{14}H_{16}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			21	14	2	4	1		

P387	K388	F389	K390	L391	T400	T409	E413	V417	W418	T419	P420	P421	I422	W423	K424	L425	W426	I434	V435	G436	A437	GLU	THR	PHE
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.80Å 111.20Å 73.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00	Depositor
% Data completeness (in resolution range)	86.3 (25.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.236 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7857	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, HEF

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	0.37	0/4544	0.91	13/6175 (0.2%)
2	B	0.36	0/3495	0.93	13/4746 (0.3%)
All	All	0.36	0/8039	0.92	26/10921 (0.2%)

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.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	221	HIS	N-CA-C	10.46	133.09	110.80
2	B	238	LYS	N-CA-C	-9.52	97.80	113.50
1	A	18	GLY	CA-C-N	6.97	126.94	119.76
1	A	18	GLY	C-N-CA	6.97	126.94	119.76
1	A	65	LYS	N-CA-C	6.95	118.81	110.19
2	B	361	HIS	N-CA-C	6.93	118.91	111.36
2	B	234	LEU	N-CA-C	6.60	118.85	110.33
2	B	237	ASP	N-CA-C	6.46	120.11	107.57
1	A	139	THR	N-CA-C	-6.37	95.72	109.81
1	A	137	ASN	N-CA-C	-6.29	102.99	111.54
1	A	137	ASN	CA-C-N	6.12	133.22	121.54
1	A	137	ASN	C-N-CA	6.12	133.22	121.54
1	A	147	ASN	N-CA-C	-6.03	106.25	113.97
1	A	175	ASN	CA-C-N	5.72	125.43	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASN	C-N-CA	5.72	125.43	119.82
1	A	132	ILE	N-CA-C	-5.66	101.94	107.55
1	A	220	LYS	N-CA-C	-5.57	98.93	110.80
2	B	147	ASN	N-CA-C	-5.57	106.41	113.43
2	B	320	ASP	CA-C-N	5.52	125.61	119.32
2	B	320	ASP	C-N-CA	5.52	125.61	119.32
2	B	237	ASP	CA-C-N	5.24	128.23	120.17
2	B	237	ASP	C-N-CA	5.24	128.23	120.17
2	B	98	ALA	N-CA-C	-5.21	106.25	113.18
2	B	391	LEU	N-CA-C	5.17	116.16	109.65
2	B	417	VAL	N-CA-C	5.03	116.14	108.80
2	B	400	THR	N-CA-C	5.02	117.64	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	232	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	4435	0	4484	124	0
2	B	3401	0	3438	100	0
3	A	21	0	16	3	0
All	All	7857	0	7938	220	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 14.

All (220) 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:139:THR:HB	1:A:140:PRO:HD3	1.30	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:VAL:O	2:B:233:GLU:HB3	1.71	0.91
1:A:136:ASN:ND2	1:A:136:ASN:H	1.69	0.90
1:A:139:THR:HB	1:A:140:PRO:CD	2.05	0.86
1:A:23:GLN:HE22	1:A:60:VAL:H	1.28	0.82
1:A:136:ASN:H	1:A:136:ASN:HD22	1.27	0.80
1:A:109:LEU:HB2	1:A:187:LEU:HB3	1.63	0.79
1:A:542:ILE:HD12	1:A:542:ILE:H	1.49	0.78
2:B:107:THR:HA	2:B:233:GLU:HG2	1.67	0.75
2:B:101:LYS:HE2	2:B:382:ILE:HG23	1.69	0.74
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.69	0.73
1:A:332:GLN:HE21	1:A:332:GLN:HA	1.55	0.72
1:A:252:TRP:HB3	1:A:257:ILE:HD11	1.71	0.71
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.71	0.71
1:A:139:THR:CB	1:A:140:PRO:HD3	2.15	0.70
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.74	0.70
1:A:138:GLU:OE2	1:A:140:PRO:HD2	1.93	0.68
1:A:132:ILE:HB	1:A:142:ILE:HB	1.78	0.65
2:B:288:ALA:O	2:B:291:GLU:HB3	1.96	0.65
2:B:13:LYS:HE2	2:B:82:LYS:O	1.97	0.65
2:B:266:TRP:CZ2	2:B:423:VAL:HG12	2.33	0.64
2:B:101:LYS:HG2	2:B:382:ILE:HA	1.80	0.63
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.80	0.63
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.81	0.62
1:A:475:GLN:HG3	1:A:476:LYS:N	2.13	0.62
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.98	0.61
2:B:266:TRP:HZ2	2:B:423:VAL:HG12	1.65	0.61
1:A:475:GLN:HG3	1:A:476:LYS:H	1.65	0.61
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.83	0.60
1:A:219:LYS:HB2	1:A:221:HIS:HD1	1.66	0.60
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.85	0.60
2:B:434:ILE:HG13	2:B:435:VAL:HG22	1.84	0.60
1:A:136:ASN:OD1	1:A:138:GLU:HG2	2.01	0.59
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.16	0.59
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.83	0.59
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.85	0.58
2:B:97:PRO:HG2	2:B:100:LEU:HD22	1.84	0.58
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.69	0.57
1:A:112:GLY:HA2	1:A:185:ASP:HB2	1.86	0.57
2:B:72:ARG:HH21	2:B:409:THR:HG22	1.70	0.57
1:A:235:HIS:HB2	1:A:238:LYS:O	2.05	0.57
1:A:359:GLY:O	1:A:514:GLU:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:THR:HG22	1:A:363:ASN:H	1.69	0.56
2:B:180:ILE:HG13	2:B:189:VAL:HG22	1.87	0.56
2:B:263:LYS:HG2	2:B:426:TRP:HE3	1.71	0.56
1:A:253:THR:O	1:A:257:ILE:HG12	2.05	0.56
1:A:270:ILE:HG23	1:A:271:TYR:CD2	2.41	0.56
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.88	0.56
1:A:441:TYR:HA	1:A:496:VAL:HG13	1.87	0.56
1:A:317:VAL:HG22	1:A:318:TYR:H	1.70	0.55
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.87	0.55
2:B:206:ARG:O	2:B:210:LEU:HD13	2.05	0.55
1:A:65:LYS:HB3	1:A:68:SER:OG	2.06	0.55
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.42	0.55
1:A:221:HIS:HD2	1:A:222:GLN:NE2	2.05	0.54
1:A:442:VAL:HG23	1:A:497:THR:HB	1.90	0.54
2:B:157:PRO:HG2	2:B:184:MET:HA	1.88	0.54
1:A:225:PRO:HB3	3:A:999:HEF:HE22	1.90	0.54
1:A:226:PRO:HA	1:A:234:LEU:O	2.08	0.53
1:A:465:LYS:HG2	1:A:466:VAL:H	1.74	0.53
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.43	0.53
2:B:233:GLU:HG3	2:B:234:LEU:CD1	2.39	0.53
2:B:233:GLU:HG3	2:B:234:LEU:HD12	1.89	0.53
2:B:22:LYS:N	2:B:22:LYS:HD2	2.24	0.53
2:B:368:LEU:O	2:B:372:VAL:HG23	2.09	0.53
1:A:193:LEU:HB3	1:A:197:GLN:HB2	1.92	0.52
2:B:388:LYS:HE3	2:B:413:GLU:HB3	1.92	0.52
1:A:100:LEU:HD21	3:A:999:HEF:H5'	1.90	0.52
1:A:208:HIS:O	1:A:212:TRP:HD1	1.92	0.52
1:A:465:LYS:HG2	1:A:466:VAL:N	2.24	0.52
1:A:11:LYS:NZ	1:A:11:LYS:HB3	2.25	0.52
1:A:134:SER:HB3	1:A:138:GLU:HB2	1.92	0.52
2:B:421:PRO:O	2:B:425:LEU:HD22	2.09	0.52
1:A:40:GLU:O	1:A:43:LYS:HG2	2.09	0.52
1:A:270:ILE:HD11	1:A:314:VAL:HG11	1.92	0.52
2:B:65:LYS:HZ3	2:B:72:ARG:HD3	1.74	0.52
1:A:28:GLU:HG2	1:A:32:LYS:HE3	1.92	0.52
2:B:258:GLN:HA	2:B:283:LEU:HD21	1.92	0.52
1:A:340:GLN:CB	1:A:351:THR:HG22	2.40	0.51
1:A:17:ASP:O	1:A:83:ARG:HD3	2.09	0.51
2:B:125:ARG:NE	2:B:147:ASN:HA	2.25	0.51
1:A:497:THR:O	1:A:535:TRP:HA	2.11	0.51
2:B:154:LYS:O	2:B:157:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:LYS:HA	2:B:374:LYS:HE2	1.93	0.51
2:B:22:LYS:HD2	2:B:22:LYS:H	1.77	0.50
1:A:3:SER:HB3	1:A:212:TRP:O	2.11	0.50
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.94	0.50
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.93	0.50
1:A:260:LEU:O	1:A:264:LEU:HD23	2.10	0.50
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.94	0.50
2:B:214:LEU:H	2:B:214:LEU:HD23	1.77	0.50
2:B:107:THR:HA	2:B:233:GLU:CG	2.38	0.50
1:A:107:THR:HG23	1:A:220:LYS:HG2	1.93	0.49
2:B:27:THR:O	2:B:31:ILE:HG13	2.12	0.49
2:B:207:GLN:HA	2:B:210:LEU:HD22	1.94	0.49
2:B:327:ALA:HA	2:B:340:GLN:O	2.13	0.49
1:A:257:ILE:O	1:A:261:VAL:HG23	2.12	0.49
1:A:376:THR:HG23	1:A:386:THR:HG22	1.95	0.49
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.95	0.49
1:A:361:HIS:HB2	1:A:510:PRO:HG3	1.94	0.49
1:A:109:LEU:HD12	1:A:216:THR:HG21	1.94	0.49
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.31	0.49
2:B:183:TYR:HB3	2:B:188:TYR:HE2	1.78	0.48
1:A:111:VAL:HG12	1:A:114:ALA:CB	2.44	0.48
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.78	0.48
1:A:49:LYS:HA	1:A:143:ARG:O	2.14	0.48
1:A:37:ILE:O	1:A:40:GLU:HB3	2.13	0.48
1:A:22:LYS:HG2	1:A:23:GLN:H	1.78	0.48
1:A:22:LYS:HG2	1:A:23:GLN:N	2.28	0.48
2:B:101:LYS:O	2:B:236:PRO:HB3	2.14	0.48
1:A:31:ILE:O	1:A:35:VAL:HG23	2.14	0.48
1:A:65:LYS:HE2	1:A:68:SER:HB3	1.96	0.47
1:A:221:HIS:CD2	1:A:222:GLN:H	2.32	0.47
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.96	0.47
2:B:96:HIS:CD2	2:B:97:PRO:O	2.67	0.47
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.96	0.47
2:B:84:THR:HB	2:B:154:LYS:HE2	1.96	0.47
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.97	0.47
2:B:175:ASN:N	2:B:176:PRO:HD3	2.30	0.47
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.96	0.47
1:A:536:VAL:HG11	1:A:542:ILE:HG21	1.97	0.47
2:B:254:VAL:HB	2:B:289:LEU:HA	1.97	0.47
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.97	0.47
1:A:135:ILE:C	1:A:137:ASN:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:O	1:A:219:LYS:HB2	2.14	0.47
2:B:198:HIS:O	2:B:202:ILE:HG12	2.15	0.47
1:A:328:GLU:HB3	1:A:340:GLN:OE1	2.14	0.46
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.15	0.46
1:A:278:GLN:O	1:A:281:LYS:HB2	2.14	0.46
1:A:334:GLN:NE2	1:A:512:GLN:HB3	2.30	0.46
1:A:490:GLY:O	1:A:528:LYS:HD2	2.15	0.46
2:B:202:ILE:O	2:B:206:ARG:HG3	2.16	0.46
1:A:379:SER:CB	1:A:387:PRO:HD3	2.45	0.46
1:A:519:ASN:O	1:A:523:GLU:HG2	2.15	0.46
1:A:104:LYS:HB3	1:A:192:ASP:HA	1.96	0.46
1:A:116:PHE:C	1:A:148:VAL:HG21	2.41	0.46
1:A:442:VAL:CG2	1:A:497:THR:HB	2.45	0.46
2:B:360:ALA:HB1	2:B:366:LYS:HB3	1.97	0.46
1:A:522:ILE:O	1:A:526:ILE:HG13	2.15	0.46
2:B:254:VAL:O	2:B:258:GLN:HG3	2.16	0.46
1:A:518:VAL:O	1:A:522:ILE:HG13	2.15	0.46
2:B:107:THR:HA	2:B:233:GLU:CB	2.46	0.46
1:A:540:LYS:HG2	2:B:280:CYS:SG	2.56	0.46
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.97	0.45
2:B:376:THR:O	2:B:380:ILE:HG13	2.16	0.45
1:A:46:LYS:HE3	1:A:116:PHE:CD2	2.50	0.45
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.31	0.45
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.97	0.45
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.97	0.45
1:A:138:GLU:CD	1:A:139:THR:H	2.25	0.45
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.99	0.45
1:A:279:LEU:HD13	1:A:302:GLU:OE1	2.16	0.45
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.80	0.45
1:A:30:LYS:HB3	1:A:71:TRP:CZ3	2.52	0.45
1:A:231:GLY:O	1:A:242:GLN:HB2	2.17	0.45
2:B:79:GLU:O	2:B:83:ARG:HG3	2.17	0.44
2:B:120:LEU:HD12	2:B:150:PRO:HD3	1.99	0.44
2:B:366:LYS:O	2:B:370:GLU:HG3	2.18	0.44
1:A:540:LYS:HB3	1:A:542:ILE:HD12	1.98	0.44
2:B:234:LEU:HD12	2:B:234:LEU:N	2.32	0.44
1:A:135:ILE:O	1:A:137:ASN:N	2.50	0.44
1:A:369:THR:HG21	1:A:409:THR:OG1	2.18	0.44
2:B:46:LYS:HE2	2:B:116:PHE:HB3	2.00	0.44
2:B:63:ILE:HD13	2:B:63:ILE:H	1.83	0.44
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ALA:HB2	2:B:214:LEU:CD1	2.45	0.44
2:B:61:PHE:N	2:B:61:PHE:CD1	2.86	0.43
2:B:379:SER:CB	2:B:387:PRO:HD3	2.48	0.43
2:B:325:LEU:HD12	2:B:343:GLN:HG2	2.01	0.43
1:A:60:VAL:HG21	1:A:130:PHE:CD1	2.53	0.43
1:A:65:LYS:CB	1:A:68:SER:OG	2.66	0.43
1:A:541:GLY:HA3	2:B:284:ARG:NH2	2.34	0.43
1:A:329:ILE:HD11	1:A:375:ILE:HD12	2.01	0.43
2:B:153:TRP:HB3	2:B:156:SER:OG	2.19	0.43
2:B:420:PRO:O	2:B:423:VAL:HG22	2.17	0.43
1:A:485:ALA:O	1:A:489:SER:HB3	2.19	0.43
2:B:66:LYS:O	2:B:67:ASP:HB2	2.19	0.43
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.84	0.43
2:B:276:VAL:HG23	2:B:279:LEU:HD12	2.01	0.43
2:B:7:THR:CG2	2:B:119:PRO:HG2	2.48	0.43
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.54	0.43
2:B:328:GLU:O	2:B:339:TYR:HA	2.19	0.43
2:B:66:LYS:HG3	2:B:67:ASP:OD1	2.19	0.42
1:A:188:TYR:CE2	3:A:999:HEF:H2'	2.54	0.42
2:B:65:LYS:HZ1	2:B:72:ARG:HE	1.66	0.42
2:B:132:ILE:HD12	2:B:132:ILE:N	2.33	0.42
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.84	0.42
2:B:328:GLU:HG2	2:B:390:LYS:CD	2.50	0.42
1:A:234:LEU:N	1:A:234:LEU:HD22	2.35	0.42
2:B:65:LYS:NZ	2:B:72:ARG:HD3	2.34	0.42
1:A:362:THR:HG22	1:A:363:ASN:N	2.34	0.42
1:A:297:GLU:HG3	1:A:298:GLU:N	2.34	0.42
2:B:163:SER:O	2:B:167:ILE:HG13	2.19	0.42
2:B:285:GLY:O	2:B:287:LYS:HG2	2.19	0.42
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.20	0.42
2:B:168:LEU:HD13	2:B:180:ILE:HG21	2.02	0.42
2:B:388:LYS:HE2	2:B:388:LYS:HB3	1.89	0.41
1:A:8:VAL:O	1:A:121:ASP:HB2	2.20	0.41
1:A:240:THR:HG22	1:A:241:VAL:N	2.35	0.41
1:A:63:ILE:O	1:A:72:ARG:HG2	2.20	0.41
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.84	0.41
1:A:358:ARG:NH1	1:A:358:ARG:HB3	2.35	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD3	1.87	0.41
1:A:181:TYR:CZ	2:B:138:GLU:HB2	2.56	0.41
1:A:331:LYS:HD2	1:A:337:TRP:CH2	2.55	0.41
1:A:221:HIS:CG	1:A:222:GLN:H	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:O	1:A:56:TYR:HA	2.21	0.41
2:B:341:ILE:N	2:B:341:ILE:HD12	2.36	0.41
2:B:105:SER:HA	2:B:234:LEU:O	2.21	0.40
2:B:197:GLN:O	2:B:201:LYS:HB2	2.21	0.40
1:A:136:ASN:C	1:A:138:GLU:N	2.78	0.40
1:A:279:LEU:HA	1:A:282:LEU:HD23	2.02	0.40
1:A:329:ILE:O	1:A:392:PRO:HD3	2.21	0.40
1:A:340:GLN:HB3	1:A:351:THR:HG22	2.02	0.40
1:A:356:ARG:HH22	1:A:371:ALA:HB2	1.86	0.40
1:A:503:LEU:HA	1:A:506:ILE:HD12	2.03	0.40
2:B:419:THR:HA	2:B:420:PRO:HD3	1.89	0.40
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.51	0.40
2:B:194:GLU:OE1	2:B:195:ILE:HG22	2.22	0.40
2:B:191:SER:OG	2:B:198:HIS:ND1	2.52	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	540/560 (96%)	486 (90%)	40 (7%)	14 (3%)	4	23
2	B	407/440 (92%)	375 (92%)	26 (6%)	6 (2%)	8	35
All	All	947/1000 (95%)	861 (91%)	66 (7%)	20 (2%)	5	27

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	138	GLU
1	A	139	THR
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	88	TRP
1	A	195	ILE
2	B	233	GLU
2	B	286	THR
1	A	140	PRO
2	B	236	PRO
2	B	358	ARG
1	A	358	ARG
1	A	489	SER
1	A	230	MET
1	A	471	ASP
2	B	232	TYR
1	A	361	HIS
2	B	97	PRO
1	A	273	GLY
1	A	111	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/499 (97%)	453 (93%)	32 (7%)	15	46
2	B	374/400 (94%)	353 (94%)	21 (6%)	19	52
All	All	859/899 (96%)	806 (94%)	53 (6%)	16	49

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	29	GLU
1	A	30	LYS
1	A	91	GLN
1	A	92	LEU
1	A	97	PRO
1	A	111	VAL

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Mol	Chain	Res	Type
1	A	136	ASN
1	A	138	GLU
1	A	195	ILE
1	A	220	LYS
1	A	221	HIS
1	A	222	GLN
1	A	237	ASP
1	A	296	THR
1	A	297	GLU
1	A	311	LYS
1	A	332	GLN
1	A	336	GLN
1	A	340	GLN
1	A	347	LYS
1	A	368	LEU
1	A	424	LYS
1	A	452	LEU
1	A	470	THR
1	A	475	GLN
1	A	480	GLN
1	A	493	VAL
1	A	496	VAL
1	A	514	GLU
1	A	540	LYS
1	A	542	ILE
2	B	22	LYS
2	B	24	TRP
2	B	61	PHE
2	B	63	ILE
2	B	122	GLU
2	B	161	GLN
2	B	197	GLN
2	B	211	ARG
2	B	233	GLU
2	B	237	ASP
2	B	240	THR
2	B	263	LYS
2	B	289	LEU
2	B	295	LEU
2	B	303	LEU
2	B	325	LEU
2	B	361	HIS

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Mol	Chain	Res	Type
2	B	366	LYS
2	B	368	LEU
2	B	386	THR
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	136	ASN
1	A	137	ASN
1	A	145	GLN
1	A	147	ASN
1	A	222	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	475	GLN
1	A	480	GLN
1	A	519	ASN
2	B	57	ASN
2	B	145	GLN
2	B	161	GLN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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
1	CSD	A	280	1	4,7,8	0.91	0	1,8,10	2.81	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	280	CSD	OD1-SG-CB	2.81	110.78	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	CA-CB-SG-OD1
1	A	280	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	HEF	A	999	-	20,22,22	1.23	2 (10%)	22,29,29	0.76	0

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
3	HEF	A	999	-	-	3/8/9/9	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	HEF	C1'-S'	3.49	1.82	1.78
3	A	999	HEF	C6-S'	3.34	1.82	1.74

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	HEF	N1-CM-OM-CE1
3	A	999	HEF	OM-CE1-CE2-OE
3	A	999	HEF	C6'-C1'-S'-C6

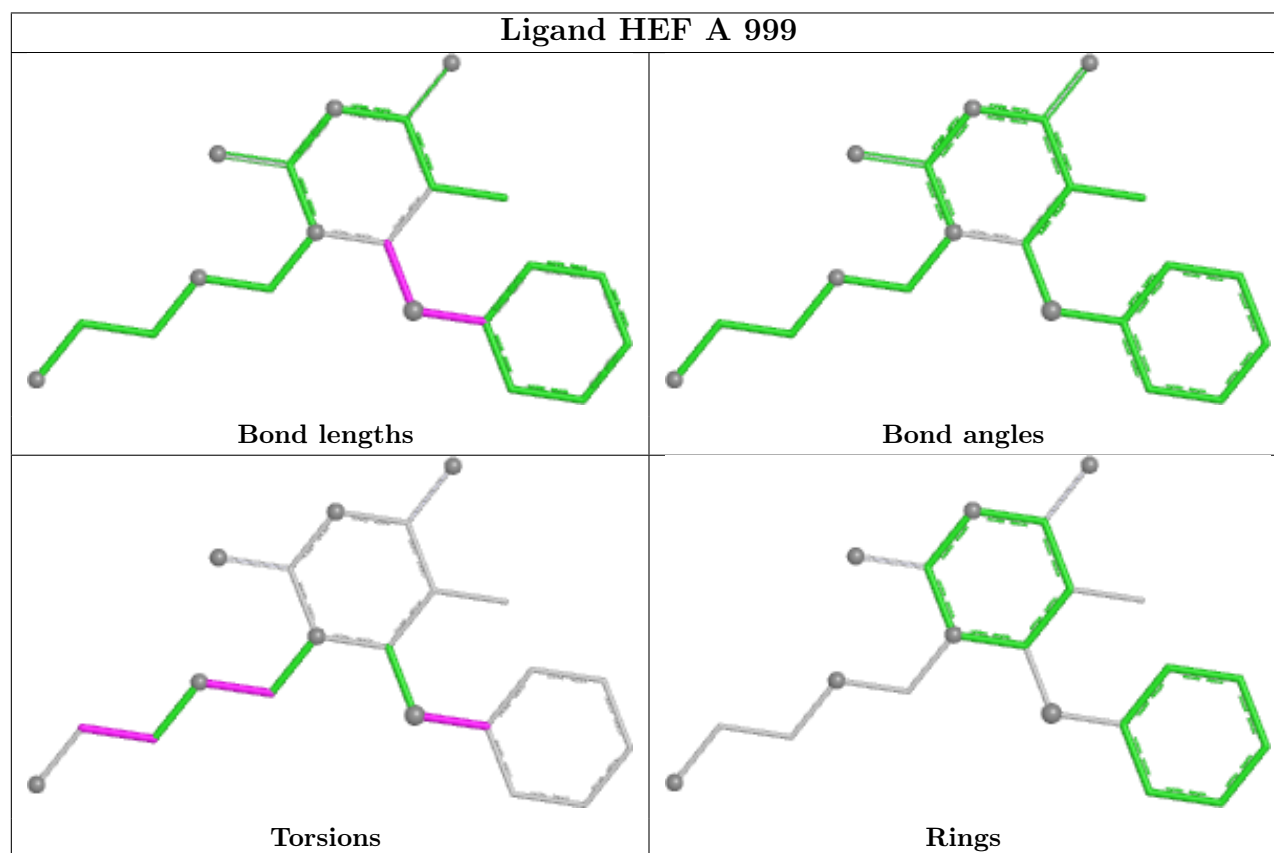
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	HEF	3	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.