Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 01:03 PM EDT

PDB ID	:	1RTI
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 (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 (1)) were used in the production of this report:

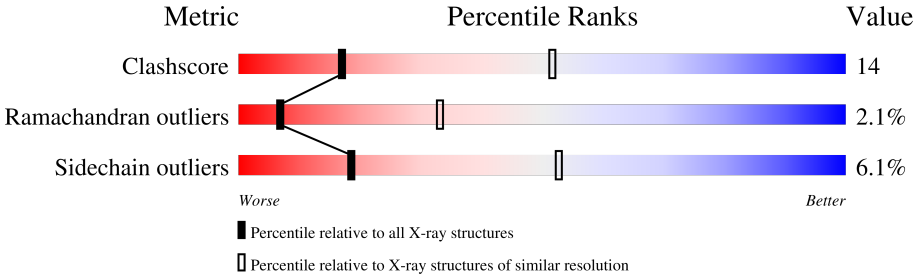
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	64% 29% • • •
2	B	440	62% 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.

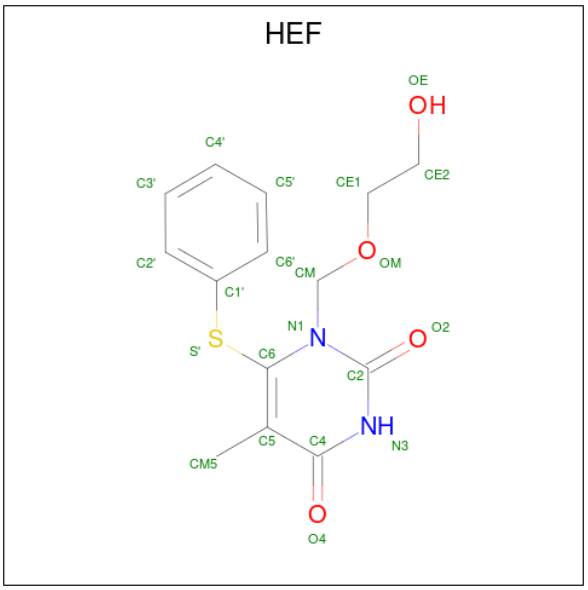
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

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

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

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

- Molecule 3 is 1-(2-HYDROXYETHYLOXYMETHYL)-6-PHENYL THIOTHYMINE (three-letter code: HEF) (formula: $C_{14}H_{16}N_2O_4S$).



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

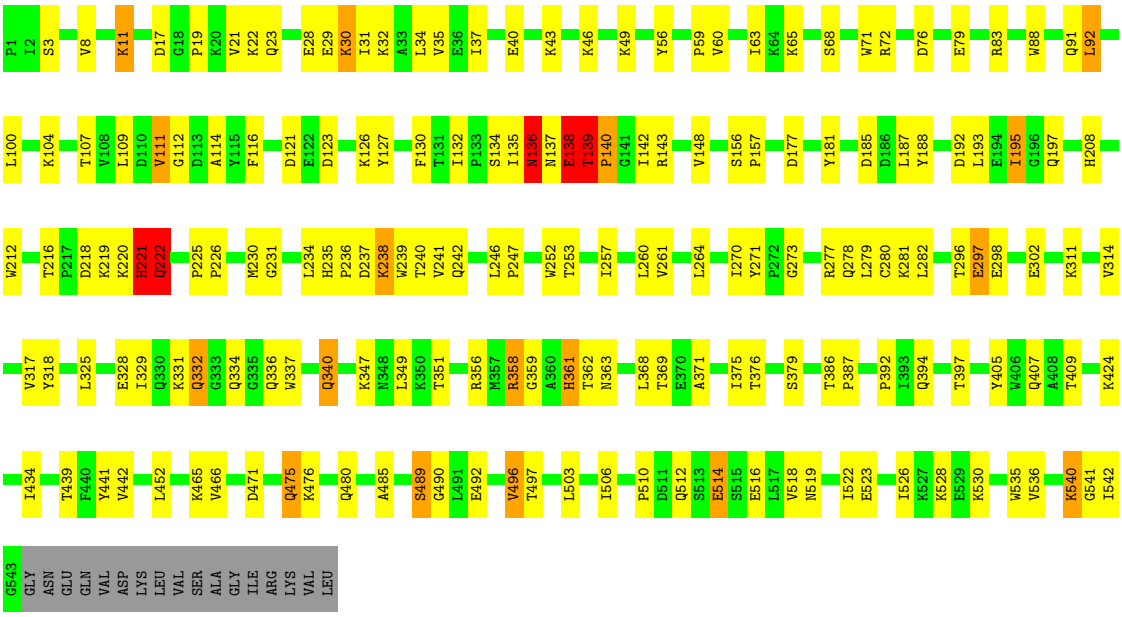
3 Residue-property plots (i)

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. 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.

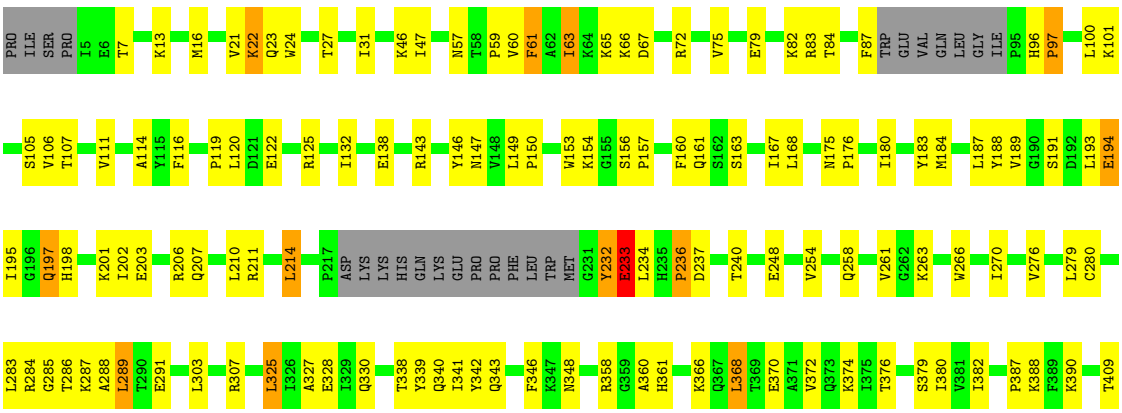
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE

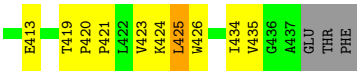
Chain A: 64% 29% • • •



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE

Chain B: 62% 29% • 6%




E413
T419
P420
P421
L422
V423
K424
L425
W426
I434
V435
G436
A437
GLU
THR
PHE

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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

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	0.30	0/4544	0.59	2/6175 (0.0%)
2	B	0.29	0/3495	0.58	0/4746
All	All	0.30	0/8039	0.59	2/10921 (0.0%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	HIS	N-CA-C	8.18	133.09	111.00
1	A	139	THR	N-CA-C	-5.66	95.72	111.00

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 (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	4435	0	4484	124	0
2	B	3401	0	3438	101	0
3	A	21	0	16	4	0
All	All	7857	0	7938	221	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 (221) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:188:TYR:HB3	3:A:999:HEF:HM51	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: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:442:VAL:CG2	1:A:497:THR:HB	2.45	0.46
2:B:65:LYS:HZ1	2:B:72:ARG:HE	1.62	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:65:LYS:HZ3	2:B:72:ARG:HD3	1.82	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
1:A:297:GLU:HG3	1:A:298:GLU:N	2.34	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: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:191:SER:OG	2:B:198:HIS:ND1	2.52	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:135:ILE:C	1:A:137:ASN:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:116:PHE:C	1:A:148:VAL:HG21	2.41	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
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
1:A:138:GLU:CD	1:A:139:THR:H	2.25	0.40
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: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
2:B:191:SER:HG	2:B:198:HIS:HD1	1.68	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

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%)	5	27
2	B	407/440 (92%)	375 (92%)	26 (6%)	6 (2%)	10	42
All	All	947/1000 (95%)	861 (91%)	66 (7%)	20 (2%)	7	33

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
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 (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	485/499 (97%)	455 (94%)	30 (6%)	18	52
2	B	374/400 (94%)	352 (94%)	22 (6%)	19	54
All	All	859/899 (96%)	807 (94%)	52 (6%)	18	53

All (52) 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	123	ASP
1	A	136	ASN
1	A	138	GLU
1	A	177	ASP
1	A	195	ILE
1	A	221	HIS
1	A	222	GLN
1	A	237	ASP
1	A	238	LYS
1	A	277	ARG
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	475	GLN
1	A	480	GLN
1	A	496	VAL
1	A	514	GLU
1	A	540	LYS
2	B	22	LYS
2	B	24	TRP
2	B	61	PHE
2	B	63	ILE
2	B	87	PHE
2	B	122	GLU
2	B	161	GLN
2	B	194	GLU
2	B	197	GLN
2	B	203	GLU
2	B	211	ARG
2	B	214	LEU

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Mol	Chain	Res	Type
2	B	233	GLU
2	B	237	ASP
2	B	240	THR
2	B	289	LEU
2	B	303	LEU
2	B	325	LEU
2	B	361	HIS
2	B	368	LEU
2	B	424	LYS
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	222	GLN
1	A	332	GLN
1	A	336	GLN
1	A	475	GLN
1	A	480	GLN
2	B	57	ASN
2	B	145	GLN
2	B	161	GLN
2	B	182	GLN
2	B	428	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)

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	3,7,8	0.64	0	1,8,10	2.76	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(^{o})	Ideal(^{o})
1	A	280	CSD	OD1-SG-CB	2.76	110.78	105.54

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 monosaccharides 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	-	22,22,22	1.15	2 (9%)	22,29,29	0.77	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'	3.31	1.82	1.78
3	A	999	HEF	C6-S'	2.96	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.

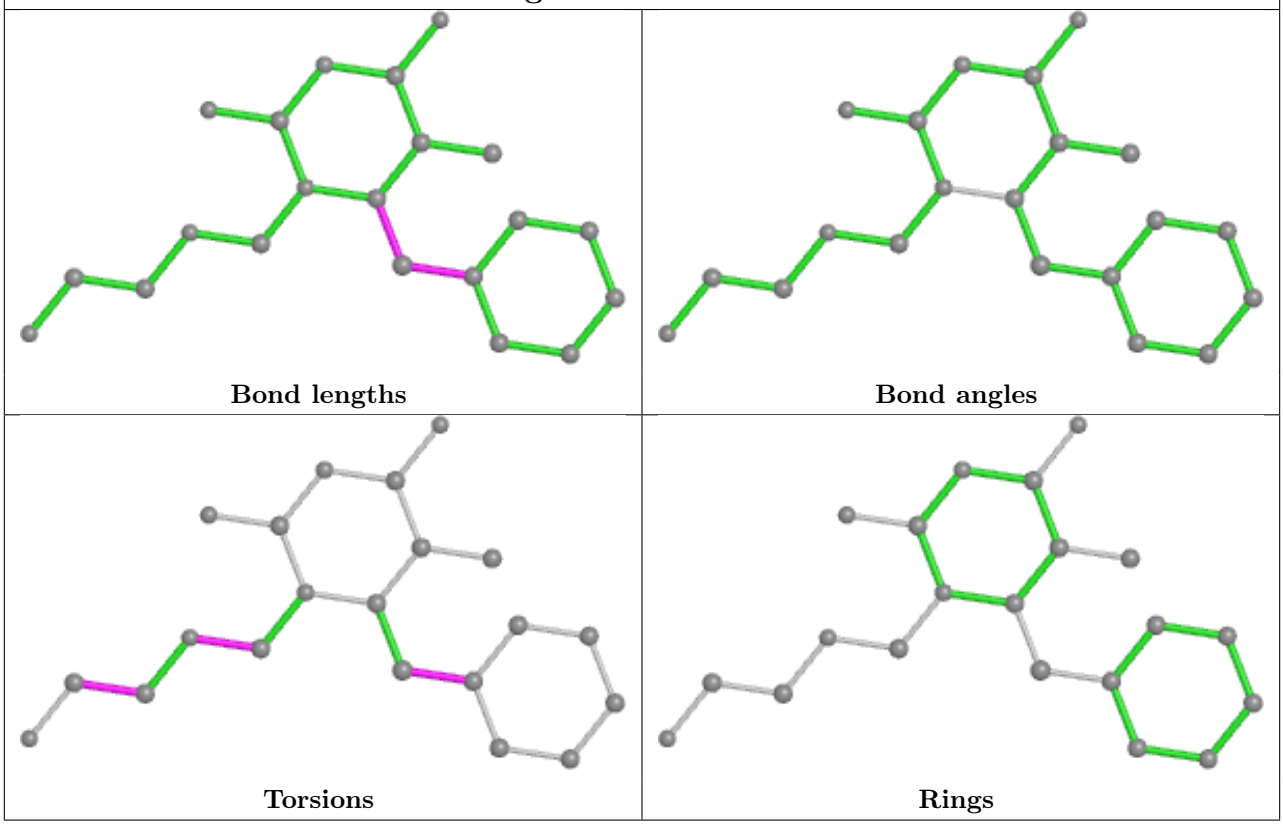
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	HEF	4	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 HEF A 999



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.