



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:02 PM GMT

PDB ID : 1RTI
Title : HIGH RESOLUTION STRUCTURES OF HIV-1 RT FROM FOUR RT-INHIBITOR COMPLEXES
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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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

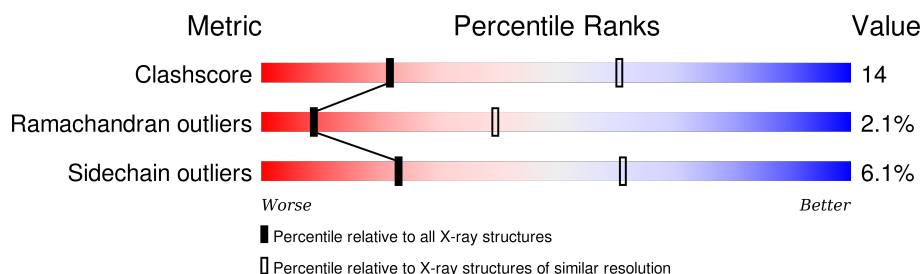
1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

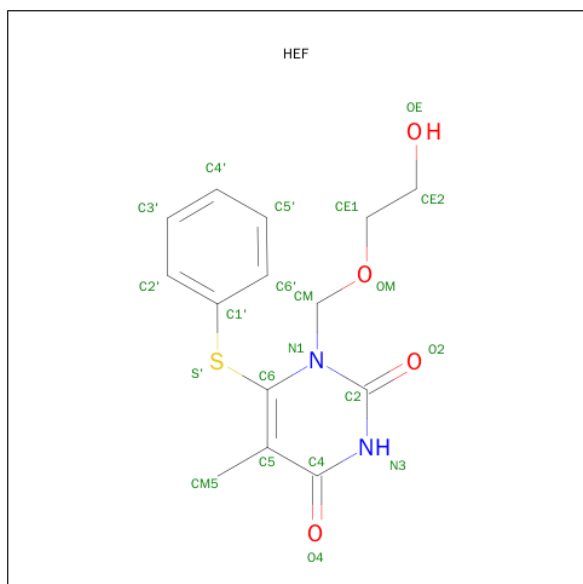
Mol	Chain	Length	Quality of chain
1	A	560	 64% 29% • • •
2	B	440	 62% 29% • 6%

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 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 THIOETHYLMINE (three-letter code: 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		

E413	T419	P420	P421	L422	V423	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 will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.80 Å 111.20 Å 73.00 Å 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	0.30	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($^{\circ}$)	Ideal($^{\circ}$)
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

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:H	1:A:136:ASN:ND2	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:HA	1:A:332:GLN:HE21	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:266:TRP:HZ2	2:B:423:VAL:HG12	1.65	0.61
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.98	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:156:SER:HB2	1:A:157:PRO:HD3	1.83	0.59
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.16	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
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:114:ALA:HB1	2:B:160:PHE:CZ	2.43	0.53
1:A:465:LYS:HG2	1:A:466:VAL:H	1.74	0.53
2:B:22:LYS:HD2	2:B:22:LYS:N	2.24	0.53
2:B:368:LEU:O	2:B:372:VAL:HG23	2.09	0.53
2:B:388:LYS:HE3	2:B:413:GLU:HB3	1.92	0.52
1:A:193:LEU:HB3	1:A:197:GLN:HB2	1.92	0.52
1:A:100:LEU:HD21	3:A:999:HEF:H5'	1.90	0.52
1:A:465:LYS:HG2	1:A:466:VAL:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:HIS:O	1:A:212:TRP:HD1	1.92	0.52
1:A:11:LYS:HB3	1:A:11:LYS:NZ	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:270:ILE:HD11	1:A:314:VAL:HG11	1.92	0.52
1:A:40:GLU:O	1:A:43:LYS:HG2	2.09	0.52
2:B:258:GLN:HA	2:B:283:LEU:HD21	1.92	0.52
1:A:28:GLU:HG2	1:A:32:LYS:HE3	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
2:B:154:LYS:O	2:B:157:PRO:HD2	2.11	0.51
1:A:497:THR:O	1:A:535:TRP:HA	2.11	0.51
2:B:374:LYS:HE2	2:B:374:LYS:HA	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
2:B:214:LEU:HD23	2:B:214:LEU:H	1.77	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: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:207:GLN:HA	2:B:210:LEU:HD22	1.94	0.49
2:B:27:THR:O	2:B:31:ILE:HG13	2.12	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:221:HIS:CD2	1:A:222:GLN:H	2.32	0.47
1:A:65:LYS:HE2	1:A:68:SER:HB3	1.96	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
1:A:188:TYR:HB3	3:A:999:HEF:HM51	1.96	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
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.15	0.46
1:A:328:GLU:HB3	1:A:340:GLN:OE1	2.14	0.46
1:A:278:GLN:O	1:A:281:LYS:HB2	2.14	0.46
2:B:202:ILE:O	2:B:206:ARG:HG3	2.16	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
1:A:519:ASN:O	1:A:523:GLU:HG2	2.15	0.46
1:A:379:SER:CB	1:A:387:PRO:HD3	2.45	0.46
1:A:442:VAL:CG2	1:A:497:THR:HB	2.45	0.46
1:A:104:LYS:HB3	1:A:192:ASP:HA	1.96	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
2:B:254:VAL:O	2:B:258:GLN:HG3	2.16	0.46
1:A:522:ILE:O	1:A:526:ILE:HG13	2.15	0.46
2:B:107:THR:HA	2:B:233:GLU:CB	2.46	0.46
1:A:518:VAL:O	1:A:522:ILE:HG13	2.15	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:HA	1:A:92:LEU:HD12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLY:O	1:A:242:GLN:HB2	2.17	0.45
1:A:30:LYS:HB3	1:A:71:TRP:CZ3	2.52	0.45
2:B:79:GLU:O	2:B:83:ARG:HG3	2.17	0.44
2:B:366:LYS:O	2:B:370:GLU:HG3	2.18	0.44
2:B:120:LEU:HD12	2:B:150:PRO:HD3	1.99	0.44
2:B:234:LEU:HD12	2:B:234:LEU:N	2.32	0.44
1:A:540:LYS:HB3	1:A:542:ILE:HD12	1.98	0.44
1:A:135:ILE:O	1:A:137:ASN:N	2.50	0.44
2:B:63:ILE:H	2:B:63:ILE:HD13	1.83	0.44
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.18	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:114:ALA:HB2	2:B:214:LEU:CD1	2.45	0.44
2:B:65:LYS:HZ3	2:B:72:ARG:HD3	1.82	0.43
2:B:61:PHE:CD1	2:B:61:PHE:N	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
2:B:72:ARG:HH11	2:B:72:ARG:HG3	1.84	0.43
1:A:485:ALA:O	1:A:489:SER:HB3	2.19	0.43
2:B:276:VAL:HG23	2:B:279:LEU:HD12	2.01	0.43
2:B:66:LYS:O	2:B:67:ASP:HB2	2.19	0.43
2:B:7:THR:CG2	2:B:119:PRO:HG2	2.48	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
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.54	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:149:LEU:HA	2:B:150:PRO:HD3	1.84	0.42
2:B:132:ILE:N	2:B:132:ILE:HD12	2.33	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
2:B:65:LYS:NZ	2:B:72:ARG:HD3	2.34	0.42
1:A:234:LEU:HD22	1:A:234:LEU:N	2.35	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
2:B:168:LEU:HD13	2:B:180:ILE:HG21	2.02	0.42
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.20	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:325:LEU:HA	1:A:325:LEU:HD23	1.84	0.41
1:A:358:ARG:HB3	1:A:358:ARG:NH1	2.35	0.41
1:A:63:ILE:O	1:A:72:ARG:HG2	2.20	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD3	1.87	0.41
1:A:331:LYS:HD2	1:A:337:TRP:CH2	2.55	0.41
1:A:181:TYR:CZ	2:B:138:GLU:HB2	2.56	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:HD12	2:B:341:ILE:N	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
2:B:191:SER:HG	2:B:198:HIS:HD1	1.68	0.40
1:A:340:GLN:HB3	1:A:351:THR:HG22	2.02	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
2:B:419:THR:HA	2:B:420:PRO:HD3	1.89	0.40
1:A:503:LEU:HA	1:A:506:ILE:HD12	2.03	0.40
1:A:356:ARG:HH22	1:A:371:ALA:HB2	1.86	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 ⓘ

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	540/560 (96%)	486 (90%)	40 (7%)	14 (3%)	7	33
2	B	407/440 (92%)	375 (92%)	26 (6%)	6 (2%)	13	50
All	All	947/1000 (95%)	861 (91%)	66 (7%)	20 (2%)	9	40

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 ⓘ

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%)	23	60
2	B	374/400 (94%)	352 (94%)	22 (6%)	24	63
All	All	859/899 (96%)	807 (94%)	52 (6%)	23	61

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

Some 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 ⓘ

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	3,7,8	0.57	0	3,8,10	2.16	1 (33%)

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	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	3.23	110.78	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	-	13,22,22	1.25	2 (15%)	13,29,29	3.48	1 (7%)

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	-	-	1/7/9/9	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'	2.47	1.82	1.77
3	A	999	HEF	C4-N3	3.42	1.39	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	HEF	C4-N3-C2	12.50	126.05	115.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	HEF	N1-C6-S'-C1'

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.