



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:35 PM EDT

PDB ID : 1FK9
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN
COMPLEX WITH DMP-266(EFAVIRENZ)
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Deposited on : 2000-08-09
Resolution : 2.50 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

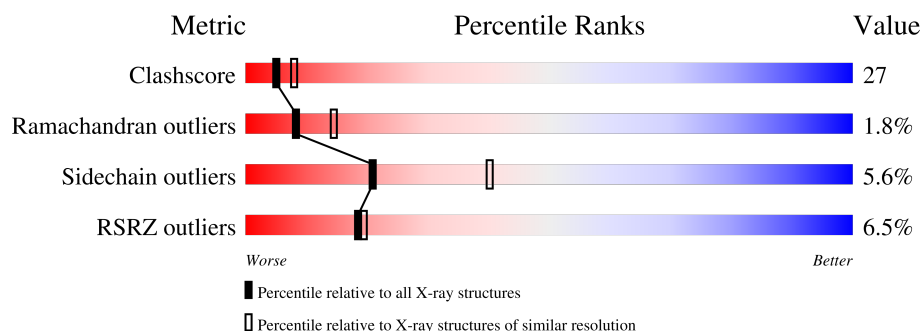
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	543	<div> <div>4%</div> <div>49%</div> <div>42%</div> <div>5%</div> <div>.</div> </div>
2	B	440	<div> <div>8%</div> <div>48%</div> <div>41%</div> <div>.</div> <div>8%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7740 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.

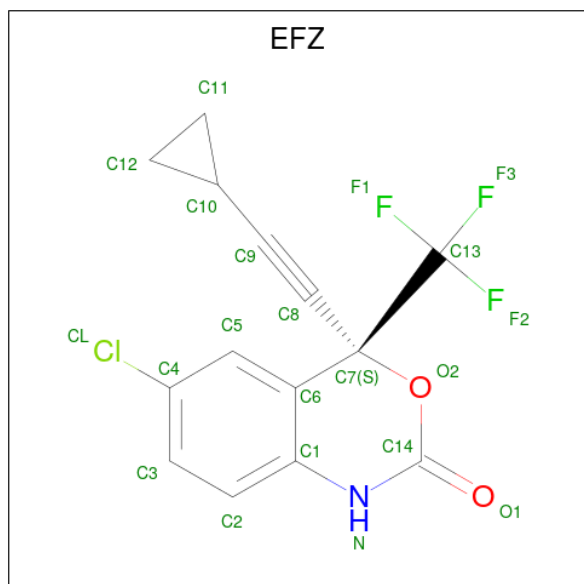
- Molecule 1 is a protein called HIV-1 RT, A-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4269	2767	706	788	8			

- Molecule 2 is a protein called HIV-1 RT, B-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3337	2172	552	607	6			

- Molecule 3 is (-)-6-CHLORO-4-CYCLOPROPYLETHYNYL-4-TRIFLUOROMETHYL-1,4-DIHYDRO-2H-3,1-BENZOXAZIN-2-ONE (three-letter code: EFZ) (formula: $C_{14}H_9ClF_3NO_2$).



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

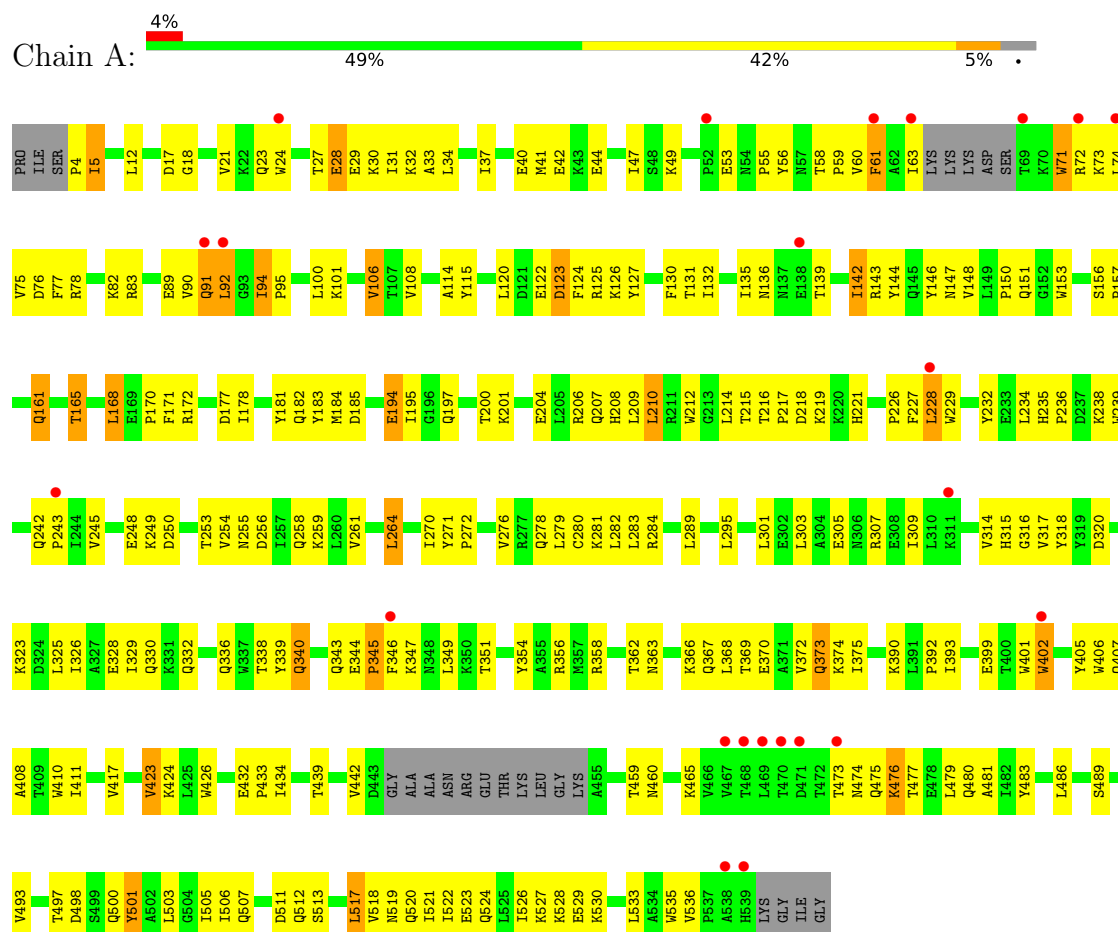
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total 63	O 63	0	0
4	B	50	Total 50	O 50	0	0

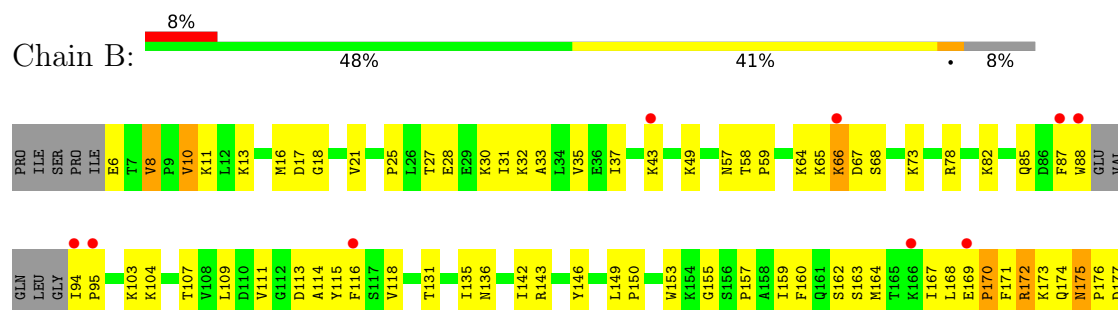
3 Residue-property plots

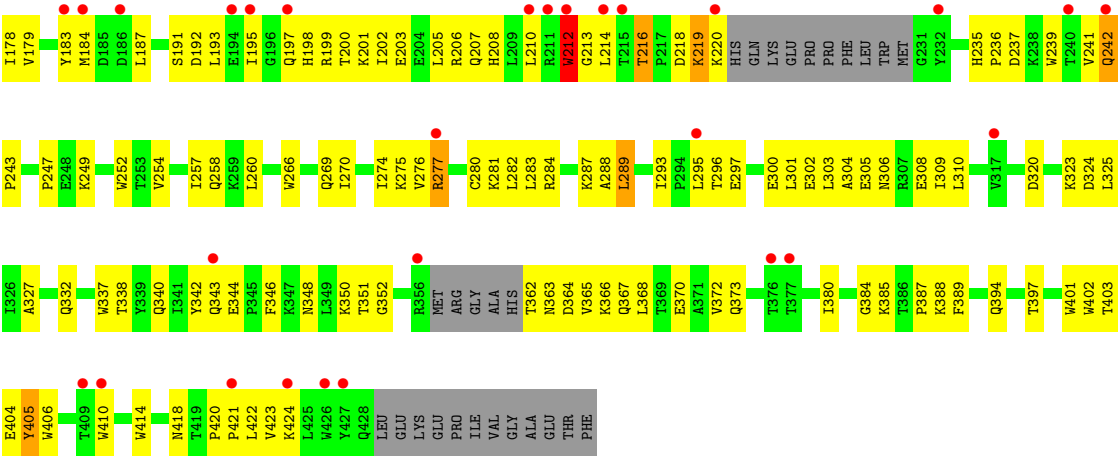
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: HIV-1 RT, A-CHAIN



• Molecule 2: HIV-1 RT, B-CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.80Å 115.00Å 65.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.2 (30.00-2.50) 85.2 (29.87-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.301 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7740	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.42	0/4375	0.64	0/5950
2	B	0.39	0/3430	0.62	0/4658
All	All	0.40	0/7805	0.63	0/10608

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4269	0	4293	245	0
2	B	3337	0	3368	180	0
3	A	21	0	9	1	0
4	A	63	0	0	7	0
4	B	50	0	0	4	0
All	All	7740	0	7670	415	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 27.

All (415) 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:111:VAL:HA	2:B:214:LEU:HD11	1.37	1.01
2:B:94:ILE:HD12	2:B:95:PRO:HD2	1.43	0.99
1:A:181:TYR:HE1	1:A:183:TYR:HB2	1.34	0.92
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.50	0.92
1:A:5:ILE:HD12	1:A:5:ILE:H	1.35	0.89
1:A:177:ASP:HA	4:A:1017:HOH:O	1.73	0.88
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.09	0.87
1:A:27:THR:HB	1:A:30:LYS:HG2	1.55	0.87
1:A:317:VAL:HG13	1:A:349:LEU:HD23	1.55	0.87
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.57	0.86
1:A:228:LEU:HD11	1:A:242:GLN:HE21	1.40	0.85
1:A:432:GLU:HG3	1:A:433:PRO:HD2	1.60	0.83
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.60	0.83
2:B:282:LEU:HG	2:B:293:ILE:HG21	1.59	0.82
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.60	0.82
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.62	0.82
1:A:356:ARG:HH21	1:A:358:ARG:NH1	1.77	0.82
1:A:332:GLN:HG2	1:A:338:THR:HG23	1.61	0.82
2:B:164:MET:SD	2:B:167:ILE:HD11	2.20	0.82
1:A:143:ARG:HB3	1:A:143:ARG:NH1	1.96	0.80
1:A:4:PRO:HG2	1:A:5:ILE:HD12	1.61	0.80
2:B:142:ILE:H	2:B:142:ILE:HD12	1.47	0.79
2:B:247:PRO:HB2	2:B:249:LYS:HD3	1.66	0.77
1:A:72:ARG:HH12	1:A:74:LEU:HD13	1.48	0.77
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.65	0.77
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.65	0.77
1:A:194:GLU:HG2	1:A:197:GLN:NE2	2.00	0.76
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.67	0.76
1:A:142:ILE:HD12	1:A:142:ILE:H	1.52	0.74
1:A:206:ARG:HH12	1:A:218:ASP:HB3	1.53	0.74
1:A:399:GLU:HG2	1:A:402:TRP:CE3	2.23	0.74
1:A:161:GLN:O	1:A:165:THR:HG23	1.88	0.73
2:B:163:SER:O	2:B:167:ILE:HG23	1.86	0.73
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.69	0.73
2:B:277:ARG:O	2:B:281:LYS:HG3	1.88	0.73
2:B:113:ASP:HB2	2:B:214:LEU:CB	2.17	0.73
2:B:254:VAL:O	2:B:258:GLN:HG3	1.88	0.72
1:A:58:THR:HG22	1:A:130:PHE:HB3	1.70	0.72
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.71	0.72
2:B:305:GLU:O	2:B:309:ILE:HG13	1.90	0.72
1:A:228:LEU:CD1	1:A:242:GLN:HE21	2.03	0.72
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASP:OD2	2:B:323:LYS:HD3	1.91	0.71
2:B:276:VAL:H	2:B:277:ARG:NH2	1.89	0.70
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.21	0.70
1:A:27:THR:HG22	1:A:29:GLU:H	1.56	0.70
1:A:132:ILE:HG13	1:A:142:ILE:HD13	1.74	0.70
1:A:301:LEU:O	1:A:305:GLU:HG3	1.91	0.69
1:A:94:ILE:HD13	1:A:94:ILE:H	1.56	0.69
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.74	0.68
1:A:206:ARG:NH1	1:A:218:ASP:HB3	2.09	0.68
2:B:66:LYS:HE2	2:B:220:LYS:HZ2	1.59	0.67
1:A:53:GLU:O	1:A:55:PRO:HD3	1.95	0.66
1:A:131:THR:HG22	1:A:143:ARG:HA	1.78	0.66
1:A:523:GLU:O	1:A:527:LYS:HG2	1.96	0.66
2:B:109:LEU:HD11	2:B:206:ARG:HH11	1.61	0.66
2:B:282:LEU:HG	2:B:293:ILE:CG2	2.26	0.66
1:A:503:LEU:O	1:A:507:GLN:HB2	1.97	0.65
1:A:136:ASN:HD22	1:A:139:THR:HG22	1.62	0.65
1:A:354:TYR:HD2	1:A:374:LYS:HD3	1.61	0.65
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.26	0.65
1:A:194:GLU:HB3	4:A:1020:HOH:O	1.97	0.65
1:A:61:PHE:N	1:A:61:PHE:HD2	1.94	0.64
1:A:399:GLU:HG2	1:A:402:TRP:HE3	1.62	0.64
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.33	0.64
2:B:113:ASP:HB2	2:B:214:LEU:HB3	1.80	0.64
1:A:524:GLN:HA	1:A:524:GLN:OE1	1.99	0.63
2:B:113:ASP:HB2	2:B:214:LEU:HB2	1.80	0.63
2:B:167:ILE:C	2:B:167:ILE:HD12	2.19	0.63
1:A:362:THR:HG22	1:A:366:LYS:HD3	1.79	0.63
2:B:340:GLN:HB3	2:B:348:ASN:HD22	1.63	0.63
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.62	0.63
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.28	0.62
1:A:58:THR:HB	4:A:1069:HOH:O	1.98	0.62
1:A:473:THR:O	1:A:477:THR:HG23	1.99	0.62
1:A:249:LYS:HE3	1:A:256:ASP:OD1	2.00	0.62
1:A:95:PRO:HB3	2:B:136:ASN:O	2.00	0.62
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.65	0.62
1:A:89:GLU:OE2	1:A:92:LEU:HD13	2.00	0.61
1:A:228:LEU:HD11	1:A:242:GLN:HG3	1.82	0.61
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.83	0.61
1:A:89:GLU:CD	1:A:92:LEU:HD13	2.21	0.61
1:A:143:ARG:HB3	1:A:143:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.36	0.60
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.15	0.60
1:A:503:LEU:HG	1:A:535:TRP:HB2	1.81	0.60
1:A:126:LYS:HE3	1:A:127:TYR:CE2	2.36	0.60
1:A:165:THR:HG22	1:A:182:GLN:HE22	1.67	0.60
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.22	0.60
2:B:164:MET:HA	2:B:167:ILE:HG13	1.83	0.60
1:A:28:GLU:O	1:A:32:LYS:HG3	2.02	0.59
2:B:332:GLN:NE2	2:B:424:LYS:HG2	2.17	0.59
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.36	0.59
1:A:255:ASN:O	1:A:259:LYS:HG2	2.03	0.59
2:B:242:GLN:NE2	2:B:352:GLY:HA2	2.18	0.59
1:A:228:LEU:HD21	1:A:242:GLN:HG3	1.85	0.59
1:A:28:GLU:HB3	1:A:32:LYS:NZ	2.18	0.58
1:A:61:PHE:N	1:A:61:PHE:CD2	2.67	0.58
1:A:432:GLU:CG	1:A:433:PRO:HD2	2.33	0.58
2:B:362:THR:HG23	2:B:366:LYS:HD3	1.85	0.58
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.37	0.58
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.85	0.58
1:A:235:HIS:HB2	1:A:238:LYS:O	2.03	0.58
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.85	0.58
1:A:228:LEU:HD13	1:A:232:TYR:O	2.04	0.58
1:A:530:LYS:HA	4:A:1036:HOH:O	2.03	0.58
1:A:73:LYS:HE2	1:A:75:VAL:CG2	2.33	0.57
1:A:101:LYS:HD2	1:A:101:LYS:N	2.19	0.57
2:B:64:LYS:NZ	2:B:66:LYS:HA	2.19	0.57
2:B:168:LEU:O	2:B:172:ARG:HB2	2.03	0.57
1:A:253:THR:CG2	1:A:256:ASP:H	2.17	0.57
2:B:203:GLU:O	2:B:206:ARG:HB2	2.04	0.57
1:A:475:GLN:O	1:A:479:LEU:HD23	2.05	0.57
1:A:354:TYR:CZ	1:A:356:ARG:HB3	2.39	0.56
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.40	0.56
1:A:253:THR:HG22	1:A:256:ASP:H	1.71	0.56
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.35	0.56
2:B:241:VAL:O	2:B:243:PRO:HD3	2.06	0.56
2:B:275:LYS:HA	2:B:277:ARG:HH21	1.71	0.56
2:B:362:THR:HG22	2:B:363:ASN:N	2.21	0.56
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.86	0.56
2:B:199:ARG:O	2:B:202:ILE:HG22	2.05	0.56
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.87	0.56
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:ND2	1:A:139:THR:HG22	2.20	0.56
2:B:31:ILE:O	2:B:35:VAL:HG23	2.07	0.56
2:B:401:TRP:O	2:B:404:GLU:HB2	2.06	0.56
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.21	0.55
1:A:37:ILE:O	1:A:41:MET:HG3	2.07	0.55
1:A:89:GLU:OE1	1:A:92:LEU:HD13	2.06	0.55
2:B:17:ASP:OD1	2:B:18:GLY:N	2.36	0.55
2:B:420:PRO:C	2:B:422:LEU:H	2.10	0.55
1:A:212:TRP:HB2	1:A:214:LEU:HD23	1.88	0.55
2:B:64:LYS:HG2	2:B:65:LYS:N	2.22	0.55
1:A:183:TYR:CD1	1:A:184:MET:HG3	2.42	0.55
1:A:183:TYR:CE1	1:A:184:MET:HG3	2.42	0.55
1:A:513:SER:HB3	1:A:519:ASN:OD1	2.07	0.55
2:B:214:LEU:HG	2:B:216:THR:HB	1.90	0.54
1:A:89:GLU:OE1	1:A:92:LEU:HB2	2.08	0.54
1:A:201:LYS:O	1:A:204:GLU:HB2	2.07	0.54
1:A:320:ASP:OD1	1:A:323:LYS:HE3	2.06	0.54
1:A:392:PRO:O	1:A:423:VAL:HG12	2.07	0.54
2:B:28:GLU:CG	2:B:32:LYS:HE3	2.37	0.54
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.35	0.54
2:B:344:GLU:OE1	2:B:344:GLU:HA	2.07	0.54
1:A:511:ASP:OD1	1:A:512:GLN:HG2	2.06	0.54
1:A:34:LEU:HD13	1:A:132:ILE:HG22	1.88	0.54
1:A:165:THR:HG22	1:A:182:GLN:NE2	2.23	0.54
1:A:406:TRP:CE3	1:A:407:GLN:HB2	2.43	0.54
2:B:11:LYS:O	2:B:85:GLN:HG2	2.08	0.54
1:A:442:VAL:CG1	1:A:481:ALA:CB	2.85	0.54
1:A:72:ARG:HH12	1:A:74:LEU:CD1	2.19	0.53
2:B:202:ILE:CG2	2:B:203:GLU:N	2.71	0.53
1:A:356:ARG:HG2	1:A:358:ARG:HG3	1.91	0.53
1:A:73:LYS:HE2	1:A:75:VAL:HG23	1.90	0.53
1:A:125:ARG:HG2	1:A:146:TYR:O	2.09	0.53
1:A:242:GLN:HG2	1:A:243:PRO:HD2	1.91	0.53
1:A:276:VAL:HG12	1:A:276:VAL:O	2.08	0.53
2:B:142:ILE:HD12	2:B:142:ILE:N	2.22	0.53
1:A:373:GLN:OE1	2:B:397:THR:HA	2.09	0.53
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.90	0.53
1:A:522:ILE:O	1:A:526:ILE:HG13	2.08	0.53
2:B:173:LYS:CA	2:B:176:PRO:HG3	2.33	0.53
1:A:183:TYR:HE1	1:A:184:MET:CE	2.21	0.52
1:A:245:VAL:HG13	1:A:245:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:C	1:A:63:ILE:HD12	2.30	0.52
1:A:314:VAL:HG22	1:A:315:HIS:N	2.24	0.52
1:A:168:LEU:O	1:A:172:ARG:HG3	2.09	0.52
1:A:264:LEU:HD23	1:A:276:VAL:HG22	1.91	0.52
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.91	0.52
1:A:363:ASN:HA	1:A:511:ASP:CG	2.30	0.52
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.90	0.52
2:B:214:LEU:H	2:B:214:LEU:HD23	1.75	0.52
2:B:169:GLU:N	2:B:170:PRO:HD2	2.25	0.52
2:B:284:ARG:HG3	2:B:287:LYS:HE3	1.91	0.52
2:B:43:LYS:HD3	4:B:1112:HOH:O	2.09	0.52
1:A:424:LYS:HE3	1:A:426:TRP:CE2	2.44	0.51
2:B:64:LYS:HZ1	2:B:66:LYS:HA	1.75	0.51
1:A:60:VAL:HG12	1:A:61:PHE:N	2.26	0.51
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.10	0.51
2:B:104:LYS:O	2:B:237:ASP:OD1	2.28	0.51
2:B:254:VAL:HB	2:B:289:LEU:O	2.10	0.51
1:A:217:PRO:HB2	1:A:221:HIS:O	2.11	0.51
1:A:340:GLN:HA	1:A:351:THR:HA	1.91	0.51
2:B:164:MET:HA	2:B:167:ILE:CG1	2.39	0.51
1:A:100:LEU:O	1:A:318:TYR:HB3	2.09	0.51
2:B:164:MET:O	2:B:167:ILE:HG13	2.10	0.51
1:A:27:THR:HG23	4:A:1003:HOH:O	2.10	0.51
1:A:33:ALA:HB2	1:A:71:TRP:CD1	2.46	0.51
1:A:56:TYR:O	1:A:143:ARG:NH2	2.43	0.51
2:B:109:LEU:HD13	2:B:218:ASP:HA	1.91	0.51
1:A:94:ILE:HG21	1:A:183:TYR:HE2	1.76	0.51
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.45	0.51
1:A:17:ASP:O	1:A:83:ARG:HD3	2.11	0.51
2:B:66:LYS:HE2	2:B:220:LYS:NZ	2.24	0.51
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.91	0.51
2:B:170:PRO:HG2	2:B:208:HIS:HE1	1.76	0.50
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.46	0.50
2:B:107:THR:HB	2:B:202:ILE:HD11	1.93	0.50
2:B:49:LYS:HB3	4:B:1054:HOH:O	2.10	0.50
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.57	0.50
2:B:282:LEU:HD21	2:B:295:LEU:HD23	1.93	0.50
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.93	0.50
1:A:210:LEU:HD21	1:A:215:THR:HG22	1.94	0.50
2:B:205:LEU:HD23	2:B:205:LEU:O	2.12	0.50
2:B:85:GLN:O	2:B:85:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ILE:H	2:B:142:ILE:CD1	2.23	0.50
1:A:183:TYR:HE1	1:A:184:MET:HE3	1.76	0.50
2:B:402:TRP:CE2	2:B:403:THR:HG23	2.47	0.50
1:A:228:LEU:HD11	1:A:242:GLN:NE2	2.17	0.49
2:B:175:ASN:HB2	2:B:177:ASP:OD1	2.12	0.49
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.42	0.49
1:A:125:ARG:NE	1:A:147:ASN:HA	2.27	0.49
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.94	0.49
1:A:497:THR:O	1:A:535:TRP:HA	2.12	0.49
2:B:350:LYS:HG2	2:B:351:THR:N	2.27	0.49
1:A:33:ALA:O	1:A:37:ILE:HG13	2.11	0.49
1:A:143:ARG:HB3	1:A:143:ARG:CZ	2.42	0.49
1:A:408:ALA:HA	2:B:364:ASP:OD1	2.13	0.49
2:B:170:PRO:HG3	2:B:212:TRP:HH2	1.78	0.49
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.48	0.49
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.95	0.48
2:B:111:VAL:CA	2:B:214:LEU:HD11	2.26	0.48
1:A:332:GLN:HG2	1:A:338:THR:CG2	2.38	0.48
1:A:210:LEU:CD2	1:A:215:THR:HG22	2.43	0.48
1:A:122:GLU:O	1:A:124:PHE:N	2.47	0.48
1:A:406:TRP:HH2	2:B:418:ASN:HD22	1.61	0.48
1:A:5:ILE:HD12	1:A:5:ILE:N	2.16	0.48
1:A:270:ILE:O	1:A:272:PRO:HD3	2.14	0.48
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.28	0.48
2:B:198:HIS:CE1	2:B:202:ILE:HD13	2.49	0.48
1:A:305:GLU:O	1:A:309:ILE:HG13	2.14	0.48
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.95	0.48
2:B:58:THR:HG23	4:B:1053:HOH:O	2.12	0.48
1:A:216:THR:HB	1:A:217:PRO:HD2	1.95	0.48
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.29	0.48
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.49	0.47
1:A:325:LEU:O	1:A:326:ILE:HD13	2.14	0.47
2:B:10:VAL:HG11	2:B:159:ILE:HD11	1.97	0.47
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.49	0.47
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.96	0.47
1:A:71:TRP:HA	1:A:71:TRP:CE3	2.49	0.47
2:B:103:LYS:O	2:B:236:PRO:HG2	2.13	0.47
2:B:380:ILE:O	2:B:384:GLY:HA2	2.13	0.47
2:B:193:LEU:HD12	2:B:197:GLN:HB3	1.95	0.47
2:B:202:ILE:HG22	2:B:203:GLU:N	2.30	0.47
2:B:266:TRP:O	2:B:269:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.49	0.47
1:A:208:HIS:O	1:A:212:TRP:CD1	2.68	0.47
2:B:284:ARG:HG3	2:B:284:ARG:O	2.15	0.47
2:B:8:VAL:HG11	2:B:159:ILE:CG2	2.44	0.47
2:B:284:ARG:O	2:B:287:LYS:HE3	2.14	0.47
2:B:302:GLU:O	2:B:306:ASN:ND2	2.47	0.47
1:A:228:LEU:HD22	1:A:232:TYR:O	2.15	0.47
1:A:229:TRP:HB3	1:A:234:LEU:CD1	2.45	0.47
1:A:278:GLN:O	1:A:282:LEU:HD13	2.15	0.47
2:B:118:VAL:HB	2:B:149:LEU:HG	1.97	0.46
2:B:324:ASP:O	2:B:343:GLN:HG2	2.15	0.46
1:A:399:GLU:O	1:A:402:TRP:HB3	2.16	0.46
1:A:410:TRP:O	1:A:411:ILE:HD13	2.15	0.46
1:A:498:ASP:HA	1:A:536:VAL:O	2.15	0.46
2:B:366:LYS:HG2	2:B:370:GLU:OE2	2.16	0.46
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.80	0.46
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.46	0.46
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.98	0.46
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.97	0.46
2:B:210:LEU:O	2:B:210:LEU:HD23	2.15	0.46
1:A:282:LEU:HD21	1:A:295:LEU:CD2	2.46	0.46
2:B:373:GLN:NE2	2:B:406:TRP:HA	2.30	0.46
1:A:94:ILE:HD13	1:A:94:ILE:N	2.26	0.46
1:A:480:GLN:CG	1:A:517:LEU:HD11	2.45	0.46
2:B:11:LYS:N	2:B:85:GLN:OE1	2.44	0.46
1:A:24:TRP:HZ3	1:A:61:PHE:CG	2.33	0.46
1:A:314:VAL:HG22	1:A:315:HIS:H	1.81	0.46
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.81	0.46
1:A:372:VAL:HG11	1:A:411:ILE:HD12	1.98	0.46
2:B:109:LEU:HB2	2:B:187:LEU:HB3	1.98	0.46
1:A:356:ARG:HE	1:A:358:ARG:HH11	1.64	0.46
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.51	0.46
2:B:167:ILE:HD12	2:B:168:LEU:HG	1.98	0.46
2:B:175:ASN:ND2	2:B:201:LYS:HD3	2.31	0.46
2:B:332:GLN:HE22	2:B:424:LYS:HG2	1.81	0.46
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.51	0.45
2:B:324:ASP:HA	2:B:385:LYS:NZ	2.31	0.45
2:B:66:LYS:HD2	2:B:67:ASP:HB2	1.98	0.45
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.46	0.45
1:A:206:ARG:NH1	1:A:218:ASP:CB	2.77	0.45
2:B:78:ARG:O	2:B:82:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASP:OD2	1:A:178:ILE:HG12	2.16	0.45
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.49	0.45
1:A:122:GLU:C	1:A:124:PHE:H	2.19	0.45
1:A:72:ARG:NH1	1:A:74:LEU:HD13	2.25	0.45
1:A:434:ILE:HA	4:A:1107:HOH:O	2.16	0.45
2:B:109:LEU:HD13	2:B:218:ASP:CA	2.47	0.45
1:A:42:GLU:OE2	1:A:49:LYS:HB2	2.17	0.45
1:A:194:GLU:HG2	1:A:197:GLN:HE21	1.78	0.45
1:A:480:GLN:O	1:A:483:TYR:HB3	2.16	0.45
1:A:524:GLN:O	1:A:528:LYS:HG2	2.16	0.45
2:B:25:PRO:HA	4:B:1047:HOH:O	2.15	0.45
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.52	0.45
2:B:170:PRO:HG2	2:B:171:PHE:H	1.82	0.45
1:A:78:ARG:O	1:A:82:LYS:HG3	2.17	0.44
1:A:303:LEU:CD2	1:A:307:ARG:HG3	2.47	0.44
1:A:236:PRO:HA	3:A:999:EFZ:H3	1.99	0.44
1:A:356:ARG:HH21	1:A:358:ARG:HH11	1.61	0.44
1:A:480:GLN:HG3	1:A:517:LEU:HD11	1.99	0.44
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.99	0.44
2:B:346:PHE:N	2:B:346:PHE:CD2	2.83	0.44
2:B:401:TRP:HE3	2:B:404:GLU:HG3	1.81	0.44
1:A:143:ARG:HH11	1:A:143:ARG:CB	2.30	0.44
1:A:270:ILE:HG23	1:A:271:TYR:N	2.32	0.44
1:A:281:LYS:O	1:A:284:ARG:HG3	2.18	0.44
1:A:363:ASN:HA	1:A:511:ASP:OD2	2.17	0.44
2:B:164:MET:CA	2:B:167:ILE:HG13	2.46	0.44
1:A:120:LEU:HB2	1:A:148:VAL:O	2.18	0.44
2:B:216:THR:HG23	2:B:216:THR:O	2.17	0.44
2:B:325:LEU:O	2:B:388:LYS:N	2.36	0.44
2:B:362:THR:CG2	2:B:363:ASN:N	2.81	0.44
1:A:344:GLU:HB3	1:A:347:LYS:HE3	1.99	0.44
1:A:473:THR:HG22	1:A:475:GLN:H	1.82	0.44
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.17	0.44
2:B:284:ARG:CG	2:B:287:LYS:HE3	2.47	0.44
1:A:170:PRO:HG2	1:A:171:PHE:H	1.82	0.44
1:A:368:LEU:HD13	1:A:368:LEU:C	2.38	0.44
2:B:327:ALA:O	2:B:389:PHE:HA	2.18	0.44
1:A:90:VAL:HG22	1:A:91:GLN:HG2	1.99	0.44
1:A:253:THR:HG22	1:A:256:ASP:CG	2.38	0.44
1:A:369:THR:HG23	1:A:411:ILE:HD11	2.00	0.43
1:A:434:ILE:HD13	1:A:530:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:THR:CG2	2:B:367:GLN:HE21	2.31	0.43
2:B:198:HIS:O	2:B:202:ILE:HB	2.18	0.43
1:A:354:TYR:OH	1:A:370:GLU:HB3	2.17	0.43
1:A:363:ASN:ND2	1:A:401:TRP:CZ3	2.85	0.43
1:A:108:VAL:HG12	1:A:227:PHE:CE1	2.53	0.43
1:A:356:ARG:NH2	1:A:358:ARG:NH1	2.58	0.43
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.54	0.43
2:B:350:LYS:CG	2:B:351:THR:N	2.81	0.43
1:A:28:GLU:HG3	1:A:135:ILE:HG12	2.00	0.43
1:A:40:GLU:HG3	1:A:44:GLU:OE1	2.18	0.43
1:A:115:TYR:N	1:A:115:TYR:CD2	2.85	0.43
1:A:399:GLU:HA	1:A:402:TRP:HB3	2.01	0.43
1:A:439:THR:O	1:A:459:THR:HA	2.19	0.43
2:B:167:ILE:CD1	2:B:168:LEU:HG	2.48	0.43
2:B:198:HIS:C	2:B:200:THR:N	2.72	0.43
1:A:131:THR:HG22	1:A:143:ARG:CA	2.47	0.43
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.54	0.43
2:B:33:ALA:O	2:B:37:ILE:HG13	2.19	0.43
1:A:27:THR:HG22	1:A:28:GLU:N	2.34	0.42
2:B:296:THR:O	2:B:297:GLU:C	2.56	0.42
1:A:142:ILE:HD12	1:A:142:ILE:N	2.27	0.42
1:A:358:ARG:NH2	2:B:394:GLN:HG3	2.34	0.42
1:A:132:ILE:HG13	1:A:142:ILE:CD1	2.45	0.42
1:A:182:GLN:NE2	4:A:1016:HOH:O	2.51	0.42
1:A:513:SER:HB2	1:A:518:VAL:HG11	2.01	0.42
1:A:332:GLN:HE21	1:A:338:THR:CG2	2.32	0.42
1:A:345:PRO:O	1:A:346:PHE:HB2	2.20	0.42
1:A:476:LYS:HG2	1:A:480:GLN:HE21	1.83	0.42
1:A:122:GLU:C	1:A:124:PHE:N	2.73	0.42
1:A:390:LYS:CB	1:A:417:VAL:HG21	2.40	0.42
2:B:13:LYS:HB2	2:B:16:MET:SD	2.60	0.42
2:B:87:PHE:CZ	2:B:155:GLY:HA2	2.55	0.42
2:B:87:PHE:O	2:B:88:TRP:HB2	2.19	0.42
2:B:195:ILE:O	2:B:199:ARG:HG3	2.20	0.42
2:B:297:GLU:O	2:B:301:LEU:HD13	2.20	0.42
1:A:27:THR:O	1:A:31:ILE:HG13	2.20	0.42
1:A:106:VAL:HG22	1:A:227:PHE:HE2	1.84	0.42
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.85	0.42
1:A:473:THR:HG22	1:A:474:ASN:N	2.34	0.42
1:A:505:ILE:HG22	1:A:506:ILE:N	2.35	0.42
2:B:103:LYS:HA	2:B:103:LYS:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLN:HE22	1:A:60:VAL:H	1.66	0.42
1:A:30:LYS:HE2	1:A:71:TRP:HH2	1.85	0.42
2:B:342:TYR:CB	2:B:348:ASN:HA	2.49	0.42
1:A:489:SER:HB2	1:A:493:VAL:HB	2.02	0.41
1:A:161:GLN:HE21	1:A:161:GLN:HB3	1.65	0.41
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.01	0.41
1:A:283:LEU:HD22	1:A:283:LEU:N	2.35	0.41
1:A:465:LYS:HZ2	1:A:465:LYS:HB2	1.85	0.41
2:B:10:VAL:CG1	2:B:159:ILE:HD11	2.50	0.41
2:B:191:SER:HB2	2:B:193:LEU:HD23	2.03	0.41
2:B:282:LEU:HD21	2:B:295:LEU:HA	2.02	0.41
2:B:372:VAL:HA	2:B:389:PHE:CE2	2.54	0.41
1:A:150:PRO:O	1:A:151:GLN:C	2.56	0.41
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.35	0.41
2:B:160:PHE:O	2:B:160:PHE:CD1	2.74	0.41
1:A:77:PHE:CE1	1:A:150:PRO:HB2	2.55	0.41
1:A:411:ILE:HD13	1:A:411:ILE:HA	1.91	0.41
2:B:173:LYS:O	2:B:176:PRO:HD3	2.20	0.41
2:B:174:GLN:C	2:B:176:PRO:HD3	2.41	0.41
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.55	0.41
1:A:108:VAL:HG13	1:A:108:VAL:O	2.21	0.41
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.55	0.41
2:B:257:ILE:HG21	2:B:283:LEU:HD13	2.02	0.41
2:B:420:PRO:HG2	2:B:423:VAL:HG23	2.03	0.41
1:A:255:ASN:OD1	1:A:259:LYS:HE2	2.21	0.41
1:A:498:ASP:OD1	1:A:498:ASP:N	2.54	0.41
2:B:199:ARG:HA	2:B:202:ILE:CG2	2.51	0.41
2:B:219:LYS:HB2	2:B:220:LYS:H	1.56	0.41
1:A:218:ASP:O	1:A:221:HIS:N	2.49	0.41
1:A:500:GLN:HB2	2:B:422:LEU:HD11	2.01	0.41
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.21	0.41
2:B:304:ALA:O	2:B:308:GLU:HB2	2.21	0.41
2:B:420:PRO:O	2:B:422:LEU:N	2.54	0.41
1:A:529:GLU:O	1:A:530:LYS:HG3	2.21	0.41
1:A:200:THR:O	1:A:204:GLU:HG3	2.21	0.40
1:A:328:GLU:O	1:A:339:TYR:HA	2.20	0.40
2:B:235:HIS:HA	2:B:236:PRO:HD2	1.89	0.40
2:B:306:ASN:HA	2:B:309:ILE:HD12	2.03	0.40
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.44	0.40
1:A:254:VAL:HG13	1:A:283:LEU:HD12	2.03	0.40
1:A:408:ALA:HB2	2:B:337:TRP:CH2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:VAL:HG13	2:B:159:ILE:HD13	2.03	0.40
2:B:282:LEU:CD2	2:B:295:LEU:HD23	2.51	0.40
2:B:303:LEU:HA	2:B:306:ASN:HD22	1.86	0.40
1:A:254:VAL:O	1:A:258:GLN:HG3	2.21	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	513/543 (94%)	461 (90%)	43 (8%)	9 (2%)	8	14
2	B	395/440 (90%)	351 (89%)	37 (9%)	7 (2%)	8	14
All	All	908/983 (92%)	812 (89%)	80 (9%)	16 (2%)	8	14

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	92	LEU
1	A	219	LYS
1	A	402	TRP
2	B	162	SER
2	B	212	TRP
2	B	216	THR
1	A	114	ALA
1	A	123	ASP
1	A	195	ILE
1	A	345	PRO
1	A	501	TYR
2	B	116	PHE
2	B	170	PRO

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Mol	Chain	Res	Type
2	B	421	PRO
2	B	213	GLY

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	468/485 (96%)	439 (94%)	29 (6%)	18	35
2	B	368/400 (92%)	350 (95%)	18 (5%)	25	47
All	All	836/885 (94%)	789 (94%)	47 (6%)	21	40

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	28	GLU
1	A	61	PHE
1	A	71	TRP
1	A	94	ILE
1	A	106	VAL
1	A	123	ASP
1	A	142	ILE
1	A	161	GLN
1	A	165	THR
1	A	168	LEU
1	A	185	ASP
1	A	194	GLU
1	A	210	LEU
1	A	228	LEU
1	A	248	GLU
1	A	250	ASP
1	A	264	LEU
1	A	279	LEU
1	A	289	LEU
1	A	336	GLN

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Mol	Chain	Res	Type
1	A	340	GLN
1	A	367	GLN
1	A	373	GLN
1	A	405	TYR
1	A	423	VAL
1	A	476	LYS
1	A	517	LEU
1	A	533	LEU
2	B	6	GLU
2	B	8	VAL
2	B	10	VAL
2	B	66	LYS
2	B	172	ARG
2	B	175	ASN
2	B	207	GLN
2	B	212	TRP
2	B	219	LYS
2	B	242	GLN
2	B	277	ARG
2	B	280	CYS
2	B	289	LEU
2	B	300	GLU
2	B	368	LEU
2	B	405	TYR
2	B	410	TRP
2	B	414	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	136	ASN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	207	GLN
1	A	222	GLN
1	A	242	GLN
1	A	278	GLN
1	A	332	GLN
1	A	475	GLN
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	507	GLN
1	A	509	GLN
1	A	520	GLN
2	B	57	ASN
2	B	147	ASN
2	B	151	GLN
2	B	175	ASN
2	B	182	GLN
2	B	255	ASN
2	B	278	GLN
2	B	332	GLN
2	B	336	GLN
2	B	407	GLN
2	B	418	ASN

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	0.77	0	1,8,10	5.00	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(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	5.00	115.05	105.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
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 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	EFZ	A	999	-	23,23,23	2.45	6 (26%)	36,36,36	1.40	2 (5%)

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	EFZ	A	999	-	-	1/10/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	EFZ	C10-C9	7.19	1.70	1.46
3	A	999	EFZ	C12-C11	-5.37	1.28	1.48
3	A	999	EFZ	C11-C10	-3.72	1.23	1.48
3	A	999	EFZ	C12-C10	-3.67	1.24	1.48
3	A	999	EFZ	C7-C6	2.90	1.55	1.51
3	A	999	EFZ	C1-N	2.35	1.43	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	EFZ	C11-C10-C9	-4.99	105.52	119.06
3	A	999	EFZ	C12-C10-C9	-4.97	105.57	119.06

There are no chirality outliers.

All (1) torsion outliers are listed below:

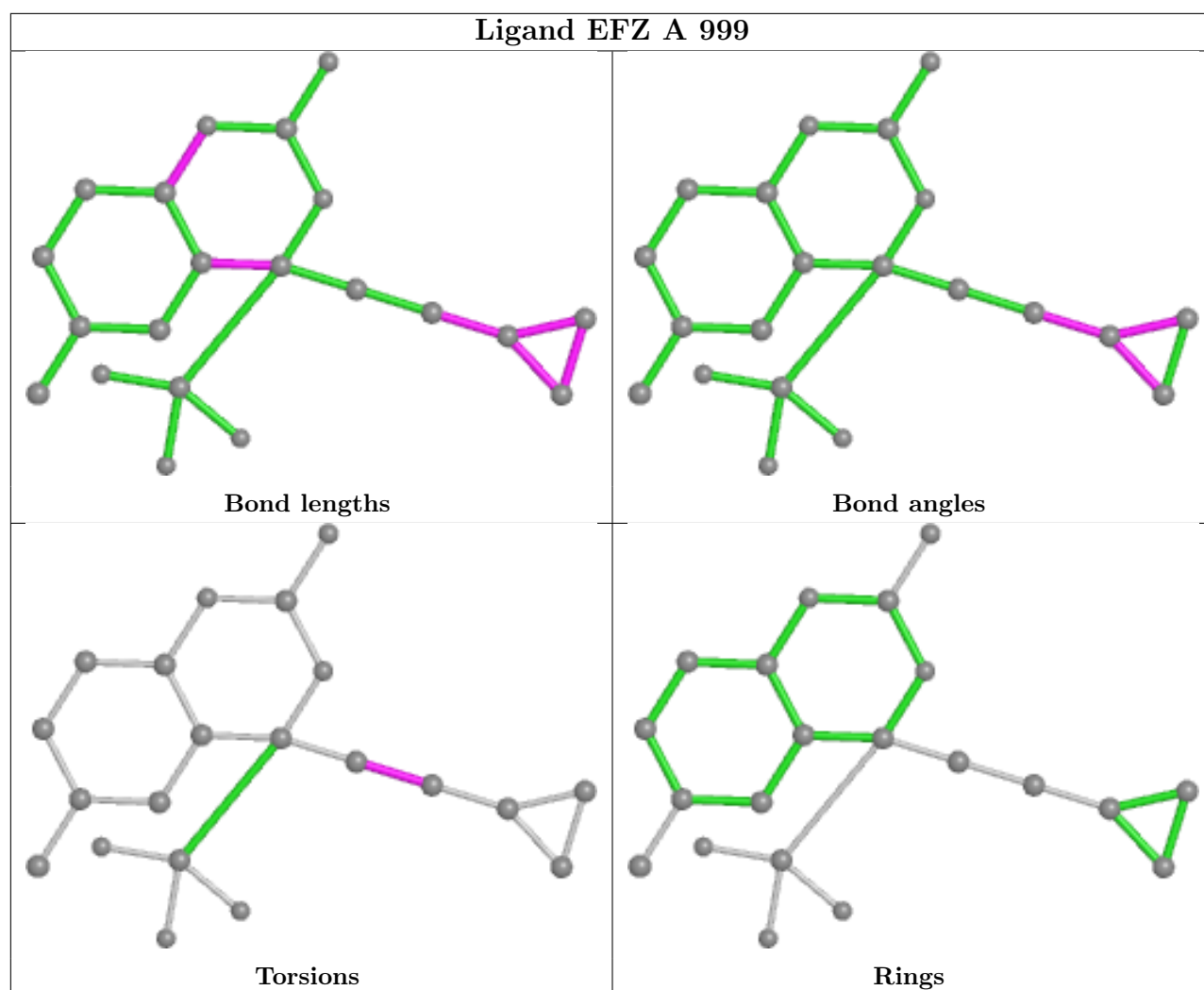
Mol	Chain	Res	Type	Atoms
3	A	999	EFZ	C7-C8-C9-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	EFZ	1	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/543 (95%)	0.02	23 (4%) 34 37	28, 63, 103, 139	0
2	B	403/440 (91%)	0.32	37 (9%) 9 9	27, 62, 111, 148	0
All	All	922/983 (93%)	0.15	60 (6%) 18 19	27, 63, 109, 148	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	21.1
1	A	402	TRP	6.1
2	B	88	TRP	5.6
2	B	211	ARG	5.5
1	A	470	THR	5.2
1	A	469	LEU	5.2
2	B	212	TRP	4.7
1	A	468	THR	4.3
1	A	63	ILE	4.3
2	B	220	LYS	4.3
1	A	471	ASP	3.9
1	A	538	ALA	3.8
2	B	410	TRP	3.7
2	B	166	LYS	3.7
2	B	356	ARG	3.4
2	B	242	GLN	3.3
2	B	184	MET	3.0
1	A	138	GLU	3.0
1	A	539	HIS	3.0
1	A	467	VAL	2.9
2	B	195	ILE	2.8
1	A	473	THR	2.8
1	A	74	LEU	2.8
2	B	424	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	169	GLU	2.7
2	B	295	LEU	2.7
2	B	66	LYS	2.6
2	B	183	TYR	2.6
2	B	194	GLU	2.6
2	B	95	PRO	2.6
2	B	215	THR	2.5
1	A	243	PRO	2.4
2	B	426	TRP	2.4
2	B	277	ARG	2.4
2	B	210	LEU	2.4
2	B	232	TYR	2.4
1	A	52	PRO	2.4
2	B	421	PRO	2.4
2	B	94	ILE	2.4
1	A	91	GLN	2.4
2	B	116	PHE	2.3
2	B	240	THR	2.3
2	B	377	THR	2.2
2	B	197	GLN	2.2
1	A	24	TRP	2.1
1	A	346	PHE	2.1
1	A	92	LEU	2.1
2	B	43	LYS	2.1
2	B	317	VAL	2.1
1	A	69	THR	2.1
2	B	409	THR	2.1
1	A	61	PHE	2.1
2	B	87	PHE	2.1
2	B	427	TYR	2.1
1	A	228	LEU	2.1
2	B	343	GLN	2.1
1	A	72	ARG	2.1
1	A	311	LYS	2.1
2	B	186	ASP	2.0
2	B	376	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSD	A	280	8/9	0.94	0.13	48,50,55,57	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

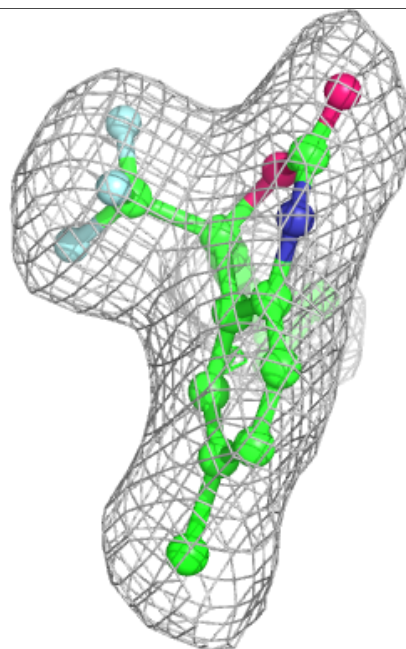
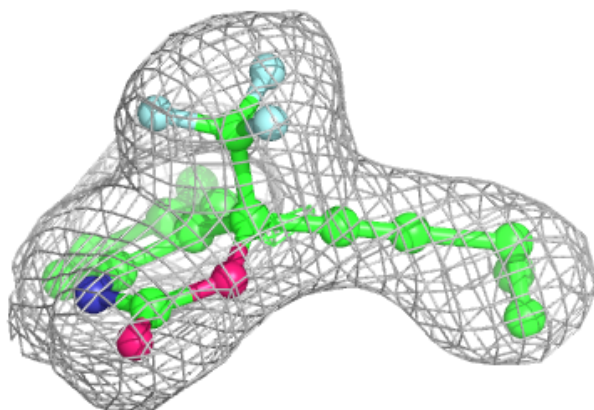
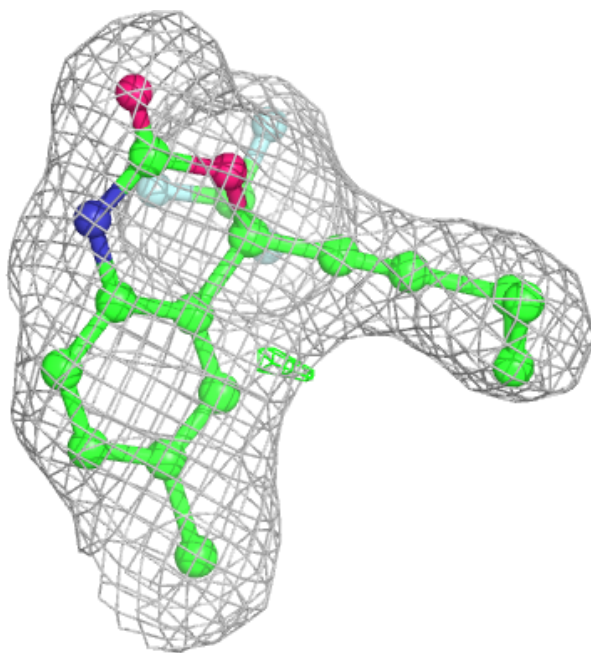
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EFZ	A	999	21/21	0.97	0.12	35,42,49,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EFZ A 999:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.