



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:33 PM UTC

PDB ID : 1IKV / pdb_00001ikv
Title : K103N Mutant HIV-1 Reverse Transcriptase in Complex with Efavirenz
Authors : Lindberg, J.; Unge, T.
Deposited on : 2001-05-07
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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

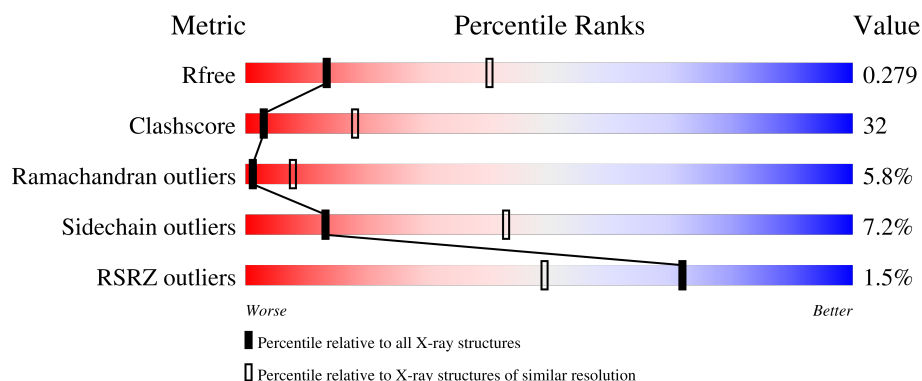
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

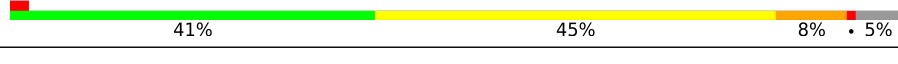
The reported resolution of this entry is 3.00 Å.

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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	560	 43% 48% 7% 2%
2	B	427	 41% 45% 8% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7872 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 POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	2	0	0
			4514	2921	752	833	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P03366
A	478	GLN	GLU	engineered mutation	UNP P03366

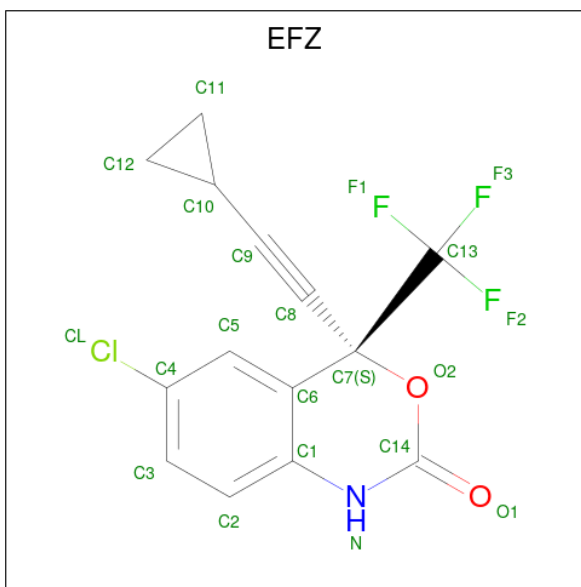
- Molecule 2 is a protein called POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	30	0	0
			3337	2174	548	609	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1103	ASN	LYS	engineered mutation	UNP P03366

- Molecule 3 is (-)-6-CHLORO-4-CYCLOPROPYLETHYNYL-4-TRIFLUOROMETHYL-1,4-DIHYDRO-2H-3,1-BENZOXAZIN-2-ONE (CCD ID: EFZ) (formula: C₁₄H₉ClF₃NO₂).



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

R1083	P1157	V1241	A1304	T1377
T1084	A1158	Q1242	E1305	E1378
Q1085	I1159	P1243	M1306	S1379
D1086	I1167	I1244	R1307	I1380
F1087	L1168	V1245	L1310	V1381
W1088	P1247	L1246	V1314	I1382
F1089	E1169	E1248	V1317	W1383
V1090	P1170	K1249	V1317	P1387
Q1091	N1175	D1250	D1320	K1388
K1102	S1251	S1251	D1320	L1391
ASN	W1252	W1252	T1263	F1392
K1104	V1254	V1254	V1263	I1393
D1110	Y1183	I1257	K1323	Q1394
V1111	M1184	I1257	D1324	L1325
G1112	D1185	Q1258	L1325	K1395
D1113	D1186	K1259	I1326	E1396
A1114	L1187	L1260	Q1330	T1397
Y1115	Y1188	V1261	G1333	W1398
F1116	V1189	G1262	Q1334	W1401
S1117	I1195	K1263	G1335	W1402
V1118	G1196	L1264	T1338	W1410
P1119	Q1197	N1265	I1341	I1411
L1120	H1198	W1266	Y1341	W1414
D1121	K1201	A1267	Y1342	E1415
E1122	I1202	Q1268	Q1343	F1416
D1123	E1203	I1270	E1344	V1417
F1124	E1204	Y1271	F1345	N1418
R1125	L1205	I1274	F1346	T1419
K1126	R1206	K1275	K1347	P1420
Y1127	L1209	Q1278	M1348	P1421
F1130	L1214	L1279	L1349	V1423
T1131	T1215	C1280	T1351	K1424
P1133	T1216	K1281	G1352	L1425
S1134	P1217	L1282	K1353	W1426
I1135	ASP	L1283	Y1354	Y1427
N1136	LYS	R1284	A1355	
E1138	LYS	G1285	A1355	
N1137	HIS	T1286	R1356	
T1139	GLN	K1287	NET	
P1140	LYS	A1288	ARG	
G1141	GLU	L1289	GLY	
I1142	PRO	T1290	ALA	
R1143	PRO	E1291	HIS	
Y1144	PHE	V1292	T1362	
Q1145	LEU	W1293	N1363	
Y1146	TRP	I1294	D1364	
N1147	NET	P1294	V1365	
V1148	G1231	L1295	V1366	
L1149	Y1232	T1296	T1369	
P1150	E1297	E1298	E1370	
Q1151	E1298	A1299	A1371	
G1152	L1234	E1300	K1374	
W1153	H1235	L1301	I1375	
K1154	P1236	E1302	T1376	
G1155	D1237	L1303		
S1156				

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.63Å 157.17Å 156.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.84 – 3.00 24.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.3 (24.84-3.00) 87.2 (24.84-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.294 0.217 , 0.279	Depositor DCC
R_{free} test set	1524 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7872	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: 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	0.51	0/4631	0.99	13/6291 (0.2%)
2	B	0.51	0/3430	1.00	22/4660 (0.5%)
All	All	0.51	0/8061	0.99	35/10951 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1293	ILE	N-CA-C	7.29	115.93	107.84
1	A	13	LYS	CA-C-N	6.90	128.47	119.84
1	A	13	LYS	C-N-CA	6.90	128.47	119.84
2	B	1235	HIS	CA-C-N	6.72	126.99	119.32
2	B	1235	HIS	C-N-CA	6.72	126.99	119.32
2	B	1298	GLU	N-CA-C	-6.72	103.42	111.69
1	A	184	MET	CB-CA-C	-6.71	108.83	116.54
2	B	1348	ASN	N-CA-C	6.54	119.21	109.59
1	A	54	ASN	CA-C-N	6.54	128.01	119.84
1	A	54	ASN	C-N-CA	6.54	128.01	119.84
2	B	1391	LEU	N-CA-C	6.31	117.60	109.65
2	B	1056	TYR	N-CA-C	6.18	119.67	110.52
1	A	225	PRO	N-CA-C	-6.17	104.55	110.47
1	A	349	LEU	N-CA-C	-6.07	106.00	113.41
2	B	1401	TRP	N-CA-C	5.99	122.04	114.31
2	B	1151	GLN	N-CA-C	5.84	120.55	112.90
2	B	1382	ILE	N-CA-C	5.83	116.05	110.74
1	A	219	LYS	N-CA-C	-5.80	106.06	114.12
2	B	1414	TRP	N-CA-C	5.76	117.77	108.32
1	A	96	HIS	N-CA-C	-5.63	101.45	109.62
2	B	1349	LEU	N-CA-C	-5.59	105.95	112.89
1	A	92	LEU	N-CA-C	-5.57	103.76	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1018	GLY	CA-C-N	5.50	125.43	119.76
2	B	1018	GLY	C-N-CA	5.50	125.43	119.76
2	B	1198	HIS	N-CA-C	-5.43	105.00	111.03
2	B	1058	THR	N-CA-C	-5.38	100.07	109.48
2	B	1351	THR	N-CA-C	-5.27	101.74	109.81
1	A	500	GLN	N-CA-C	-5.19	105.05	111.33
2	B	1081	ASN	N-CA-C	-5.17	105.54	111.07
1	A	426	TRP	N-CA-C	5.14	119.12	113.21
1	A	108	VAL	N-CA-C	5.12	115.41	107.28
2	B	1245	VAL	N-CA-C	5.05	116.52	109.80
2	B	1281	LYS	N-CA-C	-5.05	107.47	113.38
2	B	1147	ASN	N-CA-C	-5.04	107.52	113.97
2	B	1153	TRP	N-CA-C	5.02	116.45	108.67

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	4514	0	4565	296	0
2	B	3337	0	3365	225	0
3	A	21	0	8	0	0
All	All	7872	0	7938	504	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 32.

All (504) 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:223:LYS:HG3	1:A:224:GLU:H	1.05	1.09
2:B:1283:LEU:HD13	2:B:1293:ILE:HB	1.37	1.05
1:A:278:GLN:HE21	1:A:298:GLU:HB2	1.20	1.03
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1246:LEU:HD12	2:B:1307:ARG:HB3	1.47	0.93
1:A:228:LEU:HD22	1:A:242:GLN:HE21	1.32	0.92
2:B:1274:ILE:HG23	2:B:1306:ASN:HD22	1.34	0.91
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.36	0.90
1:A:223:LYS:HG3	1:A:224:GLU:N	1.87	0.89
1:A:458:VAL:HG21	1:A:547:GLN:HE22	1.37	0.89
1:A:351:THR:HG22	1:A:352:GLY:H	1.38	0.87
1:A:225:PRO:HA	1:A:226:PRO:O	1.75	0.85
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.56	0.85
1:A:485:ALA:O	1:A:489:SER:HB2	1.76	0.83
1:A:180:ILE:HG12	1:A:189:VAL:HG22	1.62	0.82
1:A:543:GLY:HA3	2:B:1284:ARG:HB3	1.59	0.82
1:A:351:THR:HG22	1:A:352:GLY:N	1.93	0.80
2:B:1365:VAL:O	2:B:1369:THR:HG23	1.81	0.80
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.64	0.79
2:B:1279:LEU:HD12	2:B:1282:LEU:HD22	1.63	0.79
1:A:543:GLY:H	2:B:1284:ARG:HD2	1.48	0.78
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.12	0.78
1:A:107:THR:HB	1:A:223:LYS:HB3	1.64	0.78
2:B:1287:LYS:HD3	2:B:1291:GLU:OE2	1.82	0.78
1:A:458:VAL:HG21	1:A:547:GLN:NE2	1.99	0.77
2:B:1249:LYS:HD2	2:B:1251:SER:HB3	1.67	0.77
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.66	0.77
2:B:1059:PRO:HG2	2:B:1076:ASP:HB3	1.67	0.77
2:B:1274:ILE:CG2	2:B:1306:ASN:HD22	1.96	0.77
2:B:1263:LYS:HE2	2:B:1425:LEU:HA	1.66	0.77
1:A:33:ALA:O	1:A:37:ILE:HG13	1.85	0.76
1:A:458:VAL:CG2	1:A:547:GLN:HE22	1.97	0.76
2:B:1013:LYS:HE3	2:B:1085:GLN:HB3	1.67	0.76
2:B:1050:ILE:CG2	2:B:1145:GLN:HG2	2.15	0.76
1:A:183:TYR:CE2	1:A:184:MET:HE2	2.20	0.76
1:A:223:LYS:CG	1:A:224:GLU:H	1.89	0.76
2:B:1247:PRO:O	2:B:1248:GLU:HG3	1.86	0.76
1:A:278:GLN:NE2	1:A:298:GLU:HB2	1.98	0.75
1:A:543:GLY:CA	2:B:1284:ARG:HB3	2.17	0.74
2:B:1254:VAL:HG12	2:B:1258:GLN:HE21	1.52	0.74
1:A:450:THR:O	1:A:451:LYS:HB2	1.88	0.73
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.70	0.73
2:B:1168:LEU:HD13	2:B:1180:ILE:HD13	1.70	0.73
1:A:26:LEU:CD2	1:A:133:PRO:HG2	2.18	0.73
1:A:351:THR:CG2	1:A:352:GLY:H	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1086:ASP:O	2:B:1090:VAL:HG22	1.89	0.73
2:B:1266:TRP:CD1	2:B:1427:TYR:HH	2.06	0.72
1:A:31:ILE:O	1:A:35:VAL:HG23	1.89	0.72
2:B:1301:LEU:O	2:B:1305:GLU:HB2	1.89	0.72
1:A:28:GLU:HG2	1:A:135:ILE:HG23	1.70	0.72
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.25	0.71
1:A:219:LYS:HD2	1:A:220:LYS:HG2	1.72	0.71
1:A:151:GLN:HE21	1:A:152:GLY:N	1.88	0.71
1:A:307:ARG:HG3	1:A:307:ARG:NH1	2.02	0.71
2:B:1231:GLY:O	2:B:1232:TYR:HB3	1.91	0.70
1:A:441:TYR:CE2	1:A:544:GLY:HA3	2.26	0.69
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.75	0.69
2:B:1203:GLU:HA	2:B:1206:ARG:HD3	1.74	0.69
1:A:518:VAL:O	1:A:522:ILE:HG13	1.92	0.69
2:B:1248:GLU:CD	2:B:1307:ARG:HH12	2.01	0.69
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.73	0.69
1:A:218:ASP:HB3	1:A:219:LYS:HE2	1.75	0.69
1:A:402:TRP:CD1	1:A:402:TRP:C	2.71	0.69
2:B:1074:LEU:HD21	2:B:1411:ILE:HD11	1.74	0.68
2:B:1156:SER:HB2	2:B:1157:PRO:HD3	1.75	0.68
1:A:151:GLN:O	1:A:153:TRP:N	2.23	0.68
2:B:1296:THR:O	2:B:1300:GLU:HG2	1.94	0.68
2:B:1169:GLU:HB3	2:B:1170:PRO:HD3	1.75	0.67
2:B:1184:MET:O	2:B:1185:ASP:HB2	1.92	0.67
1:A:426:TRP:O	1:A:427:TYR:HB3	1.92	0.67
1:A:131:THR:CG2	1:A:143:ARG:HG2	2.25	0.67
2:B:1154:LYS:HG2	2:B:1184:MET:HE2	1.77	0.67
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.75	0.66
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.76	0.66
1:A:278:GLN:HG3	1:A:298:GLU:CB	2.25	0.66
1:A:458:VAL:CB	1:A:548:VAL:HG22	2.26	0.66
1:A:27:THR:O	1:A:31:ILE:HG13	1.95	0.66
2:B:1065:LYS:HB3	2:B:1068:SER:OG	1.95	0.66
2:B:1266:TRP:CE3	2:B:1425:LEU:HD21	2.30	0.65
2:B:1122:GLU:CD	2:B:1122:GLU:H	2.03	0.65
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.27	0.64
1:A:106:VAL:HG13	1:A:225:PRO:HG2	1.79	0.64
2:B:1060:VAL:HG12	2:B:1075:VAL:HG22	1.78	0.64
2:B:1414:TRP:HD1	2:B:1414:TRP:O	1.80	0.64
1:A:139:THR:HG22	1:A:140:PRO:CD	2.26	0.64
2:B:1063:ILE:HD13	2:B:1074:LEU:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HD2	1:A:336:GLN:OE1	1.98	0.64
2:B:1253:THR:O	2:B:1257:ILE:HG22	1.98	0.64
1:A:195:ILE:HD11	1:A:199:ARG:NH2	2.12	0.64
1:A:21:VAL:CG2	1:A:79:GLU:HG3	2.28	0.63
1:A:441:TYR:O	1:A:548:VAL:HG21	1.97	0.63
1:A:44:GLU:HB2	1:A:46:LYS:HG2	1.79	0.63
2:B:1090:VAL:HG23	2:B:1091:GLN:N	2.11	0.63
2:B:1278:GLN:HB3	2:B:1298:GLU:HG3	1.80	0.63
1:A:494:ASN:HB3	2:B:1289:LEU:HD12	1.80	0.63
1:A:131:THR:HG21	1:A:143:ARG:NH1	2.14	0.62
1:A:406:TRP:CH2	2:B:1418:ASN:HA	2.34	0.62
2:B:1076:ASP:OD1	2:B:1078:ARG:HB2	1.99	0.62
1:A:218:ASP:HB3	1:A:219:LYS:CE	2.29	0.62
2:B:1031:ILE:O	2:B:1035:VAL:HG13	1.99	0.62
2:B:1073:LYS:NZ	2:B:1130:PHE:CZ	2.63	0.62
2:B:1251:SER:O	2:B:1252:TRP:HB2	1.99	0.62
2:B:1353:LYS:HG2	2:B:1354:TYR:N	2.15	0.62
1:A:458:VAL:CB	1:A:547:GLN:HE22	2.12	0.62
2:B:1268:SER:C	2:B:1270:ILE:H	2.07	0.61
1:A:466:VAL:CG2	1:A:551:LEU:HD13	2.30	0.61
1:A:64:LYS:HB3	1:A:68:SER:HA	1.83	0.61
1:A:301:LEU:O	1:A:304:ALA:HB3	2.00	0.61
2:B:1353:LYS:HG2	2:B:1354:TYR:H	1.65	0.61
2:B:1153:TRP:CE2	2:B:1155:GLY:HA3	2.36	0.61
2:B:1216:THR:HB	2:B:1217:PRO:CD	2.30	0.61
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.66	0.60
1:A:1:PRO:O	1:A:2:ILE:HG13	2.01	0.60
1:A:219:LYS:CD	1:A:220:LYS:HG2	2.32	0.60
1:A:410:TRP:CG	1:A:411:ILE:H	2.19	0.60
2:B:1275:LYS:N	2:B:1306:ASN:HD21	1.99	0.60
2:B:1279:LEU:O	2:B:1282:LEU:HB2	2.01	0.60
2:B:1296:THR:HG22	2:B:1297:GLU:OE1	2.02	0.59
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.37	0.59
2:B:1167:ILE:O	2:B:1170:PRO:HD2	2.01	0.59
1:A:26:LEU:HD23	1:A:133:PRO:HG2	1.84	0.59
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.67	0.59
1:A:497:THR:O	1:A:535:TRP:HA	2.02	0.59
2:B:1314:VAL:O	2:B:1317:VAL:HG22	2.02	0.59
2:B:1293:ILE:HD13	2:B:1293:ILE:H	1.66	0.59
1:A:101:LYS:HE3	1:A:101:LYS:N	2.17	0.59
2:B:1414:TRP:O	2:B:1414:TRP:CD1	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1005:ILE:HD11	2:B:1118:VAL:HG13	1.85	0.59
2:B:1075:VAL:HG11	2:B:1077:PHE:CZ	2.38	0.59
2:B:1417:VAL:HG22	2:B:1418:ASN:H	1.68	0.59
1:A:543:GLY:N	2:B:1284:ARG:HD2	2.17	0.58
2:B:1296:THR:HG21	2:B:1298:GLU:HG2	1.86	0.58
1:A:67:ASP:O	1:A:68:SER:HB2	2.03	0.58
2:B:1007:THR:HG22	2:B:1119:PRO:HG2	1.84	0.58
1:A:40:GLU:O	1:A:44:GLU:HG2	2.03	0.58
1:A:92:LEU:HD12	1:A:92:LEU:N	2.19	0.58
1:A:485:ALA:O	1:A:489:SER:CB	2.51	0.58
2:B:1257:ILE:O	2:B:1261:VAL:HG23	2.04	0.58
1:A:101:LYS:HE3	1:A:101:LYS:H	1.69	0.58
1:A:548:VAL:O	1:A:552:VAL:HG23	2.04	0.58
1:A:93:GLY:O	1:A:94:ILE:HD13	2.04	0.57
1:A:278:GLN:HE21	1:A:298:GLU:CB	2.07	0.57
2:B:1216:THR:HB	2:B:1217:PRO:HD2	1.87	0.57
2:B:1195:ILE:CG2	2:B:1196:GLY:N	2.66	0.57
2:B:1393:ILE:HG12	2:B:1394:GLN:N	2.19	0.57
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.35	0.57
2:B:1168:LEU:CD1	2:B:1180:ILE:HG21	2.34	0.57
1:A:107:THR:HG23	1:A:198:HIS:NE2	2.20	0.57
1:A:122:GLU:O	1:A:124:PHE:N	2.37	0.57
1:A:219:LYS:HD2	1:A:220:LYS:N	2.20	0.56
1:A:12:LEU:HB3	1:A:83:ARG:O	2.05	0.56
1:A:445:ALA:O	1:A:446:ALA:HB2	2.05	0.56
2:B:1249:LYS:CD	2:B:1251:SER:HB3	2.34	0.56
2:B:1283:LEU:HD13	2:B:1293:ILE:CB	2.26	0.56
2:B:1114:ALA:HB2	2:B:1214:LEU:HD13	1.88	0.56
1:A:225:PRO:HA	1:A:226:PRO:C	2.29	0.56
2:B:1324:ASP:O	2:B:1343:GLN:HG2	2.06	0.56
1:A:248:GLU:HA	1:A:307:ARG:NH2	2.20	0.56
1:A:451:LYS:HB3	1:A:471:ASN:HA	1.88	0.56
2:B:1209:LEU:HD22	2:B:1214:LEU:HD23	1.88	0.56
2:B:1120:LEU:O	2:B:1121:ASP:C	2.48	0.56
2:B:1280:CYS:C	2:B:1282:LEU:H	2.14	0.55
1:A:277:ARG:HG2	1:A:277:ARG:HH11	1.71	0.55
2:B:1353:LYS:NZ	2:B:1353:LYS:HB3	2.21	0.55
1:A:458:VAL:CG2	1:A:548:VAL:HG22	2.35	0.55
1:A:107:THR:CB	1:A:223:LYS:HB3	2.34	0.55
1:A:466:VAL:HG21	1:A:551:LEU:HD13	1.87	0.55
1:A:435:VAL:HG22	2:B:1290:THR:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1287:LYS:HD3	2:B:1291:GLU:CD	2.32	0.55
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.88	0.55
2:B:1422:LEU:C	2:B:1422:LEU:HD23	2.32	0.55
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.88	0.54
1:A:102:LYS:HB2	1:A:318:TYR:HB2	1.88	0.54
2:B:1023:GLN:OE1	2:B:1059:PRO:HA	2.07	0.54
2:B:1254:VAL:HG23	2:B:1291:GLU:O	2.06	0.54
2:B:1266:TRP:C	2:B:1268:SER:H	2.15	0.54
2:B:1280:CYS:C	2:B:1282:LEU:N	2.65	0.54
1:A:41:MET:HE1	1:A:73:LYS:HZ3	1.73	0.54
1:A:151:GLN:HE21	1:A:152:GLY:H	1.53	0.54
1:A:122:GLU:C	1:A:124:PHE:H	2.15	0.54
1:A:285:GLY:O	1:A:287:LYS:HG3	2.07	0.54
2:B:1363:ASN:HB3	2:B:1366:LYS:HB2	1.89	0.54
1:A:128:THR:OG1	1:A:146:TYR:HB2	2.08	0.54
2:B:1195:ILE:HG23	2:B:1196:GLY:N	2.22	0.54
2:B:1278:GLN:HB3	2:B:1298:GLU:CG	2.37	0.54
1:A:454:LYS:HE2	1:A:466:VAL:CG1	2.37	0.54
1:A:65:LYS:HG2	1:A:66:LYS:H	1.73	0.53
2:B:1168:LEU:HD13	2:B:1180:ILE:HG21	1.88	0.53
2:B:1296:THR:CG2	2:B:1298:GLU:HG2	2.38	0.53
1:A:317:VAL:HG12	1:A:348:ASN:O	2.07	0.53
1:A:458:VAL:HG11	1:A:547:GLN:NE2	2.24	0.53
2:B:1294:PRO:O	2:B:1295:LEU:HG	2.08	0.53
2:B:1251:SER:O	2:B:1252:TRP:CB	2.56	0.53
2:B:1371:ALA:O	2:B:1375:ILE:HG13	2.09	0.53
1:A:411:ILE:O	1:A:411:ILE:HG23	2.09	0.53
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.44	0.53
2:B:1304:ALA:HA	2:B:1307:ARG:HG2	1.90	0.53
1:A:248:GLU:HA	1:A:307:ARG:HH21	1.74	0.53
1:A:358:ARG:NH2	2:B:1394:GLN:HG3	2.24	0.53
1:A:410:TRP:O	1:A:411:ILE:HB	2.08	0.53
1:A:516:GLU:O	1:A:520:GLN:HG3	2.09	0.53
2:B:1090:VAL:CG2	2:B:1091:GLN:N	2.71	0.53
1:A:503:LEU:O	1:A:507:GLN:HB2	2.09	0.53
2:B:1252:TRP:HA	2:B:1252:TRP:CE3	2.43	0.53
1:A:219:LYS:HE2	1:A:219:LYS:N	2.24	0.52
1:A:125:ARG:NE	1:A:147:ASN:HA	2.24	0.52
1:A:357:MET:O	1:A:358:ARG:HB3	2.08	0.52
1:A:547:GLN:NE2	1:A:548:VAL:N	2.57	0.52
2:B:1085:GLN:HA	2:B:1088:TRP:NE1	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1252:TRP:O	2:B:1292:VAL:HG23	2.09	0.52
1:A:325:LEU:O	1:A:326:ILE:HD13	2.09	0.52
1:A:16:MET:CE	1:A:83:ARG:HG2	2.40	0.52
1:A:221:HIS:C	1:A:223:LYS:H	2.16	0.52
2:B:1296:THR:HG22	2:B:1298:GLU:H	1.75	0.52
1:A:278:GLN:NE2	1:A:298:GLU:CB	2.71	0.52
1:A:393:ILE:O	1:A:416:PHE:HD1	1.93	0.51
1:A:410:TRP:HB2	2:B:1365:VAL:HG23	1.91	0.51
2:B:1157:PRO:HG2	2:B:1184:MET:HA	1.92	0.51
2:B:1008:VAL:HG21	2:B:1159:ILE:HG23	1.91	0.51
1:A:67:ASP:O	1:A:68:SER:CB	2.58	0.51
2:B:1296:THR:HG22	2:B:1297:GLU:N	2.25	0.51
2:B:1296:THR:HG22	2:B:1297:GLU:H	1.75	0.51
2:B:1266:TRP:HB3	2:B:1427:TYR:OH	2.10	0.51
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.93	0.51
2:B:1104:LYS:HA	2:B:1237:ASP:OD1	2.11	0.51
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.91	0.50
2:B:1266:TRP:CG	2:B:1427:TYR:HH	2.30	0.50
1:A:410:TRP:CG	1:A:411:ILE:N	2.79	0.50
1:A:156:SER:N	1:A:157:PRO:CD	2.73	0.50
1:A:106:VAL:HG13	1:A:225:PRO:CG	2.40	0.50
1:A:107:THR:HA	1:A:223:LYS:CB	2.41	0.50
1:A:466:VAL:HG12	1:A:466:VAL:O	2.11	0.50
1:A:122:GLU:C	1:A:124:PHE:N	2.68	0.50
1:A:257:ILE:O	1:A:261:VAL:HG23	2.11	0.50
1:A:410:TRP:HE3	1:A:410:TRP:HA	1.77	0.50
1:A:458:VAL:HG21	1:A:547:GLN:CD	2.36	0.50
2:B:1320:ASP:OD2	2:B:1323:LYS:HG3	2.11	0.50
1:A:295:LEU:HB3	1:A:300:GLU:HG2	1.94	0.50
1:A:551:LEU:HD12	1:A:552:VAL:HG23	1.94	0.50
1:A:53:GLU:H	1:A:53:GLU:CD	2.18	0.50
1:A:476:LYS:O	1:A:480:GLN:N	2.45	0.50
1:A:134:SER:O	1:A:135:ILE:C	2.55	0.49
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.43	0.49
1:A:435:VAL:HG22	2:B:1290:THR:HG21	1.93	0.49
2:B:1268:SER:C	2:B:1270:ILE:N	2.69	0.49
1:A:120:LEU:HD12	1:A:121:ASP:N	2.27	0.49
1:A:355:ALA:O	1:A:356:ARG:C	2.55	0.49
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.47	0.49
1:A:297:GLU:O	1:A:301:LEU:HD13	2.13	0.49
1:A:469:LEU:HD22	1:A:472:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1267:ALA:O	2:B:1274:ILE:HG13	2.11	0.49
2:B:1307:ARG:HA	2:B:1310:LEU:HD12	1.94	0.49
1:A:3:SER:HB2	1:A:212:TRP:O	2.12	0.49
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.94	0.49
1:A:458:VAL:HB	1:A:548:VAL:CG2	2.36	0.49
2:B:1064:LYS:O	2:B:1065:LYS:O	2.31	0.49
1:A:543:GLY:HA3	2:B:1284:ARG:CB	2.36	0.49
2:B:1151:GLN:O	2:B:1185:ASP:OD1	2.31	0.49
2:B:1261:VAL:HG21	2:B:1284:ARG:NH2	2.27	0.49
2:B:1396:GLU:OE1	2:B:1396:GLU:N	2.32	0.49
1:A:252:TRP:HE3	1:A:256:ASP:HB3	1.78	0.49
1:A:277:ARG:HD2	1:A:336:GLN:CD	2.38	0.49
2:B:1047:ILE:HD12	2:B:1144:TYR:CD1	2.47	0.49
2:B:1266:TRP:O	2:B:1268:SER:N	2.45	0.49
1:A:206:ARG:CZ	1:A:217:PRO:O	2.61	0.49
1:A:131:THR:CG2	1:A:143:ARG:NH1	2.76	0.48
2:B:1028:GLU:HG3	2:B:1135:ILE:HD11	1.94	0.48
2:B:1282:LEU:O	2:B:1283:LEU:C	2.56	0.48
1:A:26:LEU:HD22	1:A:133:PRO:HG2	1.95	0.48
1:A:111:VAL:HG21	1:A:164:MET:CE	2.43	0.48
2:B:1024:TRP:CG	2:B:1025:PRO:HD2	2.48	0.48
1:A:151:GLN:CD	1:A:151:GLN:H	2.22	0.48
1:A:343:GLN:HG3	1:A:349:LEU:HD12	1.94	0.48
1:A:361:HIS:HD2	1:A:513:SER:OG	1.96	0.48
1:A:389:PHE:HB3	1:A:391:LEU:CD2	2.38	0.48
1:A:351:THR:CG2	1:A:352:GLY:N	2.59	0.48
2:B:1262:GLY:O	2:B:1265:ASN:HB3	2.14	0.48
2:B:1275:LYS:O	2:B:1306:ASN:ND2	2.47	0.48
2:B:1064:LYS:NZ	2:B:1069:THR:HA	2.29	0.48
2:B:1374:LYS:O	2:B:1378:GLU:HG3	2.14	0.48
1:A:454:LYS:O	1:A:552:VAL:HG13	2.14	0.47
1:A:90:VAL:HG13	1:A:161:GLN:HG3	1.95	0.47
1:A:406:TRP:CH2	1:A:407:GLN:OE1	2.66	0.47
2:B:1260:LEU:HD22	2:B:1279:LEU:HD21	1.95	0.47
1:A:498:ASP:HB2	1:A:538:ALA:HA	1.96	0.47
1:A:109:LEU:CD1	1:A:205:LEU:HD23	2.45	0.47
1:A:458:VAL:HG11	1:A:547:GLN:CD	2.40	0.47
2:B:1293:ILE:HD13	2:B:1293:ILE:N	2.29	0.47
1:A:203:GLU:OE2	1:A:206:ARG:HD3	2.14	0.47
2:B:1154:LYS:CG	2:B:1184:MET:HE2	2.42	0.47
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ALA:HA	1:A:72:ARG:O	2.14	0.47
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.30	0.47
2:B:1115:TYR:C	2:B:1117:SER:H	2.23	0.47
2:B:1427:TYR:O	2:B:1427:TYR:CD1	2.68	0.47
2:B:1023:GLN:HG2	2:B:1133:PRO:HD3	1.95	0.47
2:B:1050:ILE:HG23	2:B:1145:GLN:HG2	1.95	0.47
2:B:1215:THR:HG22	2:B:1216:THR:H	1.79	0.47
2:B:1417:VAL:HG22	2:B:1418:ASN:N	2.29	0.47
1:A:325:LEU:C	1:A:326:ILE:HD13	2.40	0.47
2:B:1060:VAL:CG1	2:B:1075:VAL:HG22	2.43	0.47
1:A:222:GLN:O	1:A:223:LYS:C	2.58	0.46
2:B:1153:TRP:CZ2	2:B:1155:GLY:HA3	2.50	0.46
2:B:1275:LYS:C	2:B:1306:ASN:HD21	2.23	0.46
1:A:253:THR:HA	1:A:292:VAL:HA	1.97	0.46
2:B:1231:GLY:O	2:B:1232:TYR:CB	2.62	0.46
1:A:295:LEU:HB2	1:A:300:GLU:OE2	2.15	0.46
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.96	0.46
1:A:397:THR:HG21	1:A:424:LYS:HA	1.98	0.46
2:B:1283:LEU:CD1	2:B:1293:ILE:HB	2.27	0.46
1:A:240:THR:OG1	1:A:241:VAL:N	2.48	0.46
1:A:254:VAL:O	1:A:258:GLN:HG3	2.15	0.46
1:A:21:VAL:HG21	1:A:79:GLU:HG3	1.97	0.46
1:A:151:GLN:HB2	1:A:152:GLY:H	1.61	0.46
2:B:1047:ILE:HA	2:B:1145:GLN:O	2.16	0.46
2:B:1058:THR:HG21	2:B:1077:PHE:CD1	2.50	0.46
2:B:1139:THR:O	2:B:1140:PRO:C	2.58	0.46
1:A:470:THR:O	1:A:471:ASN:HB2	2.15	0.46
1:A:346:PHE:N	1:A:346:PHE:CD2	2.79	0.46
2:B:1330:GLN:HE21	2:B:1330:GLN:HB2	1.58	0.46
1:A:499:SER:HB3	1:A:502:ALA:HB3	1.98	0.46
2:B:1234:LEU:C	2:B:1236:PRO:HD3	2.41	0.46
2:B:1281:LYS:C	2:B:1284:ARG:HG2	2.41	0.46
2:B:1296:THR:HB	2:B:1299:ALA:CB	2.46	0.46
1:A:173:LYS:HD3	1:A:173:LYS:C	2.40	0.45
1:A:128:THR:HG21	1:A:150:PRO:HG2	1.97	0.45
1:A:175:ASN:C	1:A:177:ASP:H	2.23	0.45
1:A:223:LYS:O	1:A:224:GLU:C	2.58	0.45
2:B:1110:ASP:C	2:B:1112:GLY:H	2.25	0.45
2:B:1154:LYS:O	2:B:1157:PRO:HD2	2.16	0.45
2:B:1275:LYS:N	2:B:1306:ASN:ND2	2.63	0.45
1:A:17:ASP:O	1:A:83:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:OE1	1:A:49:LYS:NZ	2.44	0.45
1:A:275:LYS:HE2	1:A:332:GLN:OE1	2.16	0.45
2:B:1266:TRP:CD2	2:B:1425:LEU:HD11	2.51	0.45
1:A:194:GLU:O	1:A:196:GLY:N	2.50	0.45
2:B:1037:ILE:O	2:B:1041:MET:HG3	2.15	0.45
2:B:1183:TYR:CD2	2:B:1380:ILE:HD13	2.52	0.45
2:B:1335:GLY:O	2:B:1355:ALA:HA	2.17	0.45
1:A:107:THR:HG22	1:A:223:LYS:HE3	1.99	0.45
1:A:224:GLU:O	1:A:225:PRO:C	2.60	0.45
1:A:438:GLU:HG2	1:A:459:THR:HB	1.97	0.45
1:A:467:VAL:HG22	1:A:484:LEU:HD11	1.99	0.45
2:B:1344:GLU:O	2:B:1347:LYS:HB2	2.16	0.45
1:A:489:SER:OG	1:A:493:VAL:HB	2.17	0.45
2:B:1326:ILE:O	2:B:1341:ILE:HA	2.17	0.45
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.52	0.45
1:A:171:PHE:CD1	1:A:171:PHE:C	2.95	0.45
2:B:1258:GLN:NE2	2:B:1289:LEU:HD23	2.31	0.45
1:A:9:PRO:HA	1:A:121:ASP:CG	2.42	0.45
1:A:309:ILE:O	1:A:309:ILE:HG22	2.17	0.45
1:A:361:HIS:CD2	1:A:513:SER:OG	2.69	0.45
1:A:447:ASN:HB3	1:A:450:THR:HB	1.99	0.45
2:B:1081:ASN:ND2	2:B:1154:LYS:HG3	2.31	0.45
2:B:1254:VAL:O	2:B:1258:GLN:HG3	2.16	0.45
2:B:1084:THR:O	2:B:1084:THR:HG22	2.16	0.45
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.52	0.44
2:B:1401:TRP:O	2:B:1402:TRP:C	2.60	0.44
1:A:339:TYR:CE2	1:A:375:ILE:HG12	2.52	0.44
1:A:445:ALA:O	1:A:477:THR:HG21	2.17	0.44
2:B:1274:ILE:CG2	2:B:1306:ASN:ND2	2.74	0.44
2:B:1325:LEU:HD13	2:B:1383:TRP:CE3	2.52	0.44
1:A:41:MET:HE1	1:A:73:LYS:NZ	2.32	0.44
1:A:219:LYS:CD	1:A:219:LYS:H	2.31	0.44
1:A:434:ILE:HG21	1:A:492:GLU:HB3	2.00	0.44
2:B:1017:ASP:O	2:B:1083:ARG:NH1	2.49	0.44
2:B:1066:LYS:O	2:B:1067:ASP:HB2	2.17	0.44
2:B:1353:LYS:CG	2:B:1354:TYR:H	2.31	0.44
1:A:210:LEU:C	1:A:212:TRP:H	2.25	0.44
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.00	0.44
1:A:454:LYS:HE2	1:A:466:VAL:HG11	1.99	0.44
1:A:129:ALA:HA	1:A:144:TYR:O	2.17	0.44
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1258:GLN:NE2	2:B:1289:LEU:CD2	2.80	0.44
1:A:219:LYS:HD2	1:A:219:LYS:H	1.82	0.44
2:B:1038:CYS:SG	2:B:1132:ILE:HD11	2.57	0.44
1:A:77:PHE:O	1:A:78:ARG:C	2.60	0.44
1:A:111:VAL:HG21	1:A:164:MET:HE3	2.00	0.44
1:A:182:GLN:HE21	1:A:182:GLN:HB2	1.67	0.44
2:B:1124:PHE:CD1	2:B:1127:TYR:HD2	2.35	0.44
2:B:1266:TRP:HB3	2:B:1427:TYR:HH	1.82	0.44
1:A:520:GLN:C	1:A:522:ILE:N	2.75	0.43
1:A:524:GLN:O	1:A:527:LYS:N	2.43	0.43
2:B:1115:TYR:HB3	2:B:1149:LEU:HB2	1.99	0.43
1:A:202:ILE:O	1:A:205:LEU:HB3	2.18	0.43
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.33	0.43
2:B:1050:ILE:HG21	2:B:1145:GLN:HG2	1.95	0.43
2:B:1189:VAL:HG21	2:B:1205:LEU:CD2	2.48	0.43
2:B:1353:LYS:CG	2:B:1354:TYR:N	2.82	0.43
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.83	0.43
1:A:544:GLY:N	2:B:1285:GLY:O	2.51	0.43
2:B:1090:VAL:CG2	2:B:1091:GLN:H	2.30	0.43
2:B:1252:TRP:HA	2:B:1252:TRP:HE3	1.83	0.43
1:A:12:LEU:O	1:A:13:LYS:C	2.61	0.43
1:A:390:LYS:C	1:A:391:LEU:HD23	2.43	0.43
2:B:1013:LYS:CE	2:B:1085:GLN:HB3	2.45	0.43
2:B:1168:LEU:O	2:B:1169:GLU:C	2.61	0.43
1:A:6:GLU:HG3	1:A:7:THR:N	2.33	0.43
1:A:130:PHE:CD1	1:A:130:PHE:N	2.85	0.43
1:A:50:ILE:O	1:A:143:ARG:HB2	2.18	0.43
1:A:219:LYS:CE	1:A:219:LYS:H	2.31	0.43
1:A:494:ASN:OD1	1:A:532:TYR:HB3	2.19	0.43
1:A:520:GLN:O	1:A:523:GLU:HG3	2.18	0.43
2:B:1303:LEU:O	2:B:1307:ARG:HG2	2.19	0.43
1:A:194:GLU:C	1:A:196:GLY:N	2.76	0.43
1:A:412:PRO:HG3	2:B:1401:TRP:CZ2	2.54	0.43
1:A:487:GLN:C	1:A:489:SER:H	2.27	0.43
2:B:1064:LYS:HZ2	2:B:1069:THR:HA	1.82	0.43
2:B:1252:TRP:O	2:B:1292:VAL:HA	2.18	0.43
2:B:1267:ALA:HB1	2:B:1310:LEU:HD21	2.00	0.43
1:A:218:ASP:HB3	1:A:219:LYS:HE3	2.01	0.43
1:A:254:VAL:HG22	1:A:293:ILE:HD11	2.01	0.43
1:A:178:ILE:HD13	1:A:191:SER:HB3	2.00	0.43
1:A:442:VAL:HG21	1:A:482:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1215:THR:HG22	2:B:1216:THR:N	2.34	0.43
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.53	0.42
2:B:1125:ARG:NH1	2:B:1147:ASN:OD1	2.52	0.42
1:A:38:CYS:HA	1:A:41:MET:HE3	2.00	0.42
1:A:254:VAL:HG23	1:A:291:GLU:O	2.19	0.42
1:A:492:GLU:HA	1:A:530:LYS:O	2.19	0.42
1:A:498:ASP:HB2	1:A:538:ALA:CA	2.49	0.42
2:B:1280:CYS:SG	2:B:1281:LYS:N	2.92	0.42
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.54	0.42
1:A:437:ALA:O	1:A:438:GLU:O	2.37	0.42
1:A:497:THR:OG1	1:A:498:ASP:N	2.51	0.42
2:B:1035:VAL:HG12	2:B:1132:ILE:HG21	2.01	0.42
2:B:1330:GLN:NE2	2:B:1338:THR:OG1	2.51	0.42
1:A:219:LYS:HE2	1:A:219:LYS:H	1.85	0.42
1:A:437:ALA:O	1:A:438:GLU:C	2.62	0.42
2:B:1284:ARG:HA	2:B:1284:ARG:HD3	1.85	0.42
1:A:248:GLU:CA	1:A:307:ARG:HH21	2.32	0.42
1:A:460:ASN:ND2	2:B:1288:ALA:HB2	2.35	0.42
2:B:1344:GLU:O	2:B:1345:PRO:C	2.63	0.42
1:A:110:ASP:O	1:A:110:ASP:CG	2.61	0.42
2:B:1271:TYR:O	2:B:1274:ILE:HG12	2.19	0.42
2:B:1290:THR:O	2:B:1291:GLU:C	2.63	0.42
1:A:81:ASN:OD1	1:A:153:TRP:HD1	2.02	0.42
1:A:120:LEU:HD12	1:A:121:ASP:H	1.85	0.42
1:A:203:GLU:OE2	1:A:206:ARG:NH1	2.50	0.42
1:A:410:TRP:HB2	2:B:1365:VAL:CG2	2.49	0.42
2:B:1419:THR:HA	2:B:1420:PRO:HD3	1.82	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.55	0.42
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.19	0.42
2:B:1369:THR:HG22	2:B:1398:TRP:CZ3	2.55	0.42
2:B:1376:THR:HB	2:B:1410:TRP:CH2	2.55	0.42
2:B:1388:LYS:NZ	2:B:1415:GLU:OE1	2.48	0.42
2:B:1393:ILE:CG1	2:B:1394:GLN:N	2.82	0.42
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.50	0.42
1:A:520:GLN:C	1:A:522:ILE:H	2.27	0.42
2:B:1112:GLY:C	2:B:1114:ALA:N	2.78	0.42
2:B:1187:LEU:HA	2:B:1187:LEU:HD23	1.81	0.41
1:A:221:HIS:C	1:A:223:LYS:N	2.77	0.41
1:A:23:GLN:CG	1:A:133:PRO:HG3	2.51	0.41
1:A:398:TRP:NE1	1:A:402:TRP:HE3	2.18	0.41
2:B:1154:LYS:C	2:B:1157:PRO:HD2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1278:GLN:HB2	2:B:1302:GLU:OE2	2.21	0.41
1:A:105:SER:O	1:A:190:GLY:HA2	2.19	0.41
1:A:171:PHE:CE1	1:A:205:LEU:HD13	2.55	0.41
1:A:258:GLN:HG2	1:A:283:LEU:HD13	2.01	0.41
1:A:84:THR:HG22	1:A:85:GLN:N	2.36	0.41
1:A:151:GLN:HE21	1:A:151:GLN:C	2.29	0.41
1:A:458:VAL:HG21	1:A:547:GLN:OE1	2.19	0.41
2:B:1064:LYS:HZ3	2:B:1069:THR:C	2.29	0.41
1:A:257:ILE:HB	1:A:283:LEU:HD21	2.02	0.41
2:B:1139:THR:O	2:B:1139:THR:HG22	2.20	0.41
2:B:1241:VAL:O	2:B:1243:PRO:HD3	2.20	0.41
2:B:1249:LYS:HG2	2:B:1250:ASP:N	2.35	0.41
2:B:1286:THR:HG22	2:B:1286:THR:O	2.19	0.41
1:A:93:GLY:HA3	2:B:1137:ASN:ND2	2.35	0.41
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.46	0.41
1:A:339:TYR:CG	1:A:375:ILE:HD11	2.55	0.41
1:A:522:ILE:O	1:A:523:GLU:C	2.63	0.41
2:B:1019:PRO:HG2	2:B:1080:LEU:HB2	2.02	0.41
2:B:1060:VAL:HG12	2:B:1075:VAL:HA	2.02	0.41
2:B:1279:LEU:HD12	2:B:1282:LEU:CD2	2.42	0.41
1:A:228:LEU:HD13	1:A:242:GLN:NE2	2.35	0.41
1:A:324:ASP:O	1:A:343:GLN:HG2	2.21	0.41
1:A:442:VAL:HG11	1:A:485:ALA:HB2	2.03	0.41
1:A:513:SER:OG	1:A:514:GLU:N	2.53	0.41
2:B:1085:GLN:O	2:B:1086:ASP:C	2.63	0.41
2:B:1333:GLY:O	2:B:1334:GLN:HB2	2.20	0.41
1:A:75:VAL:O	1:A:77:PHE:N	2.53	0.41
1:A:210:LEU:C	1:A:212:TRP:N	2.79	0.41
1:A:332:GLN:HB3	1:A:333:GLY:H	1.46	0.41
2:B:1249:LYS:HB3	2:B:1252:TRP:CZ3	2.56	0.41
2:B:1423:VAL:O	2:B:1424:LYS:C	2.64	0.41
1:A:489:SER:HB3	1:A:528:LYS:NZ	2.36	0.40
2:B:1379:SER:CB	2:B:1387:PRO:HD3	2.51	0.40
1:A:2:ILE:O	1:A:2:ILE:HG22	2.20	0.40
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.21	0.40
2:B:1278:GLN:O	2:B:1282:LEU:HD13	2.21	0.40
1:A:201:LYS:HB2	1:A:201:LYS:HE2	1.89	0.40
1:A:382:ILE:O	2:B:1136:ASN:HB2	2.22	0.40
1:A:397:THR:C	1:A:400:THR:HG22	2.46	0.40
2:B:1047:ILE:O	2:B:1047:ILE:HG13	2.21	0.40
2:B:1175:ASN:OD1	2:B:1201:LYS:NZ	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1298:GLU:CG	2:B:1299:ALA:N	2.85	0.40
2:B:1142:ILE:H	2:B:1142:ILE:HG13	1.64	0.40
1:A:130:PHE:O	1:A:131:THR:HG23	2.21	0.40
1:A:245:VAL:HG13	1:A:245:VAL:O	2.22	0.40
1:A:320:ASP:HA	1:A:321:PRO:HD3	1.93	0.40
1:A:354:TYR:OH	1:A:356:ARG:HB3	2.20	0.40
2:B:1081:ASN:HD22	2:B:1154:LYS:HE3	1.86	0.40
2:B:1244:ILE:HD13	2:B:1427:TYR:CD2	2.57	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	552/560 (99%)	438 (79%)	78 (14%)	36 (6%)	1	5
2	B	396/427 (93%)	333 (84%)	44 (11%)	19 (5%)	2	11
All	All	948/987 (96%)	771 (81%)	122 (13%)	55 (6%)	1	8

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ILE
2	B	1065	LYS
2	B	1252	TRP
2	B	1267	ALA
2	B	1294	PRO
1	A	2	ILE
1	A	5	ILE
1	A	18	GLY
1	A	68	SER
1	A	76	ASP

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Mol	Chain	Res	Type
1	A	123	ASP
1	A	151	GLN
1	A	152	GLY
1	A	223	LYS
1	A	230	MET
1	A	250	ASP
1	A	286	THR
1	A	427	TYR
1	A	433	PRO
1	A	438	GLU
1	A	451	LYS
2	B	1136	ASN
2	B	1184	MET
2	B	1247	PRO
2	B	1248	GLU
2	B	1251	SER
2	B	1283	LEU
1	A	268	SER
1	A	332	GLN
1	A	446	ALA
2	B	1140	PRO
2	B	1291	GLU
1	A	66	LYS
1	A	78	ARG
1	A	195	ILE
1	A	226	PRO
1	A	345	PRO
1	A	412	PRO
1	A	437	ALA
2	B	1018	GLY
2	B	1113	ASP
2	B	1116	PHE
2	B	1345	PRO
1	A	14	PRO
1	A	358	ARG
1	A	411	ILE
2	B	1232	TYR
1	A	224	GLU
2	B	1111	VAL
2	B	1133	PRO
1	A	217	PRO
1	A	417	VAL

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Mol	Chain	Res	Type
1	A	466	VAL
1	A	537	PRO
1	A	556	ILE

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	494/500 (99%)	453 (92%)	41 (8%)	10	37
2	B	368/389 (95%)	347 (94%)	21 (6%)	18	52
All	All	862/889 (97%)	800 (93%)	62 (7%)	13	43

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	14	PRO
1	A	53	GLU
1	A	101	LYS
1	A	102	LYS
1	A	106	VAL
1	A	113	ASP
1	A	135	ILE
1	A	145	GLN
1	A	151	GLN
1	A	174	GLN
1	A	179	VAL
1	A	182	GLN
1	A	185	ASP
1	A	215	THR
1	A	216	THR
1	A	219	LYS
1	A	234	LEU
1	A	240	THR
1	A	251	SER

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Mol	Chain	Res	Type
1	A	260	LEU
1	A	280	CYS
1	A	290	THR
1	A	307	ARG
1	A	325	LEU
1	A	332	GLN
1	A	345	PRO
1	A	349	LEU
1	A	357	MET
1	A	362	THR
1	A	373	GLN
1	A	402	TRP
1	A	404	GLU
1	A	410	TRP
1	A	417	VAL
1	A	432	GLU
1	A	488	ASP
1	A	491	LEU
1	A	517	LEU
1	A	523	GLU
1	A	547	GLN
2	B	1035	VAL
2	B	1039	THR
2	B	1042	GLU
2	B	1058	THR
2	B	1074	LEU
2	B	1078	ARG
2	B	1122	GLU
2	B	1139	THR
2	B	1187	LEU
2	B	1252	TRP
2	B	1266	TRP
2	B	1293	ILE
2	B	1297	GLU
2	B	1330	GLN
2	B	1345	PRO
2	B	1353	LYS
2	B	1369	THR
2	B	1370	GLU
2	B	1422	LEU
2	B	1425	LEU
2	B	1426	TRP

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

Mol	Chain	Res	Type
1	A	54	ASN
1	A	136	ASN
1	A	145	GLN
1	A	151	GLN
1	A	182	GLN
1	A	221	HIS
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	361	HIS
1	A	407	GLN
1	A	524	GLN
1	A	545	ASN
1	A	547	GLN
2	B	1081	ASN
2	B	1137	ASN
2	B	1161	GLN
2	B	1182	GLN
2	B	1258	GLN
2	B	1306	ASN
2	B	1332	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	2000	-	23,23,23	4.36	12 (52%)	36,36,36	1.85	10 (27%)

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	2000	-	-	4/10/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	EFZ	C4-CL	-16.68	1.35	1.74
3	A	2000	EFZ	C9-C8	5.51	1.35	1.19
3	A	2000	EFZ	C7-C6	5.00	1.58	1.51
3	A	2000	EFZ	C5-C6	4.01	1.45	1.39
3	A	2000	EFZ	C1-C6	3.49	1.44	1.40
3	A	2000	EFZ	C14-N	3.46	1.42	1.35
3	A	2000	EFZ	C3-C2	3.16	1.43	1.38
3	A	2000	EFZ	C5-C4	3.06	1.43	1.38
3	A	2000	EFZ	C13-C7	2.98	1.60	1.53
3	A	2000	EFZ	C3-C4	2.77	1.43	1.38
3	A	2000	EFZ	C2-C1	2.34	1.43	1.39
3	A	2000	EFZ	C12-C11	2.22	1.56	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	EFZ	C12-C10-C9	-4.10	109.42	119.09
3	A	2000	EFZ	O2-C7-C13	3.59	111.29	104.78
3	A	2000	EFZ	C7-O2-C14	-3.54	115.21	121.48
3	A	2000	EFZ	O2-C14-N	3.25	122.41	117.14
3	A	2000	EFZ	O2-C7-C6	2.97	113.84	111.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	EFZ	C4-C5-C6	2.90	122.27	118.38
3	A	2000	EFZ	O2-C7-C8	-2.84	101.91	108.32
3	A	2000	EFZ	C11-C10-C9	2.65	125.33	119.09
3	A	2000	EFZ	F3-C13-C7	-2.50	108.78	111.80
3	A	2000	EFZ	C5-C6-C7	2.45	125.47	122.69

There are no chirality outliers.

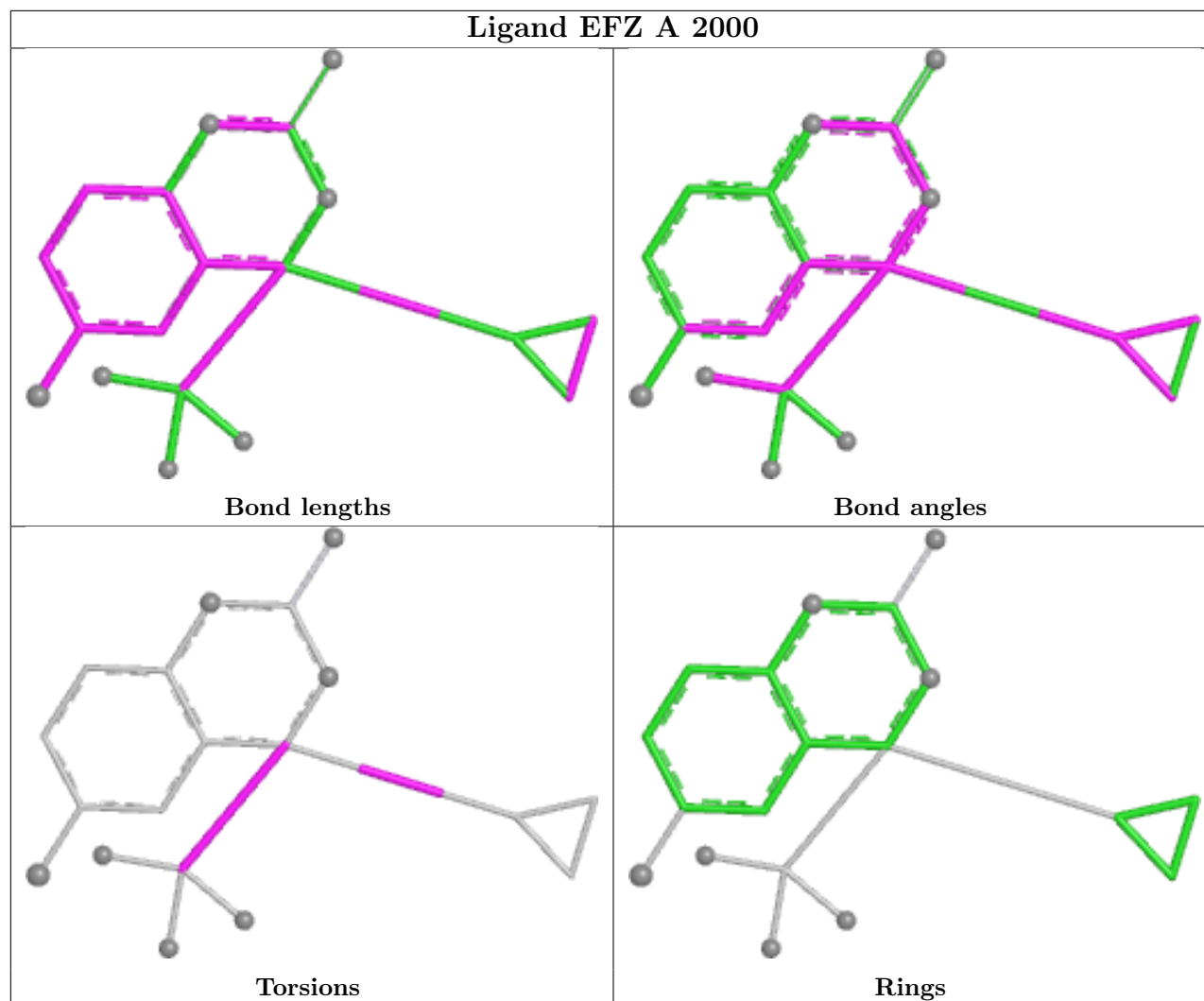
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2000	EFZ	F1-C13-C7-O2
3	A	2000	EFZ	C7-C8-C9-C10
3	A	2000	EFZ	F3-C13-C7-O2
3	A	2000	EFZ	F2-C13-C7-O2

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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

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	556/560 (99%)	-0.20	7 (1%)	75 53	13, 52, 88, 125	2 (0%)
2	B	404/427 (94%)	-0.25	7 (1%)	69 45	14, 43, 106, 122	9 (2%)
All	All	960/987 (97%)	-0.22	14 (1%)	72 49	13, 48, 99, 125	11 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1427	TYR	3.7
1	A	539	HIS	3.6
2	B	1283	LEU	3.4
2	B	1253	THR	3.0
1	A	446	ALA	2.8
1	A	151	GLN	2.6
1	A	19	PRO	2.6
1	A	447	ASN	2.6
2	B	1217	PRO	2.5
2	B	1271	TYR	2.5
1	A	18	GLY	2.2
1	A	458	VAL	2.1
2	B	1299	ALA	2.0
2	B	1215	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

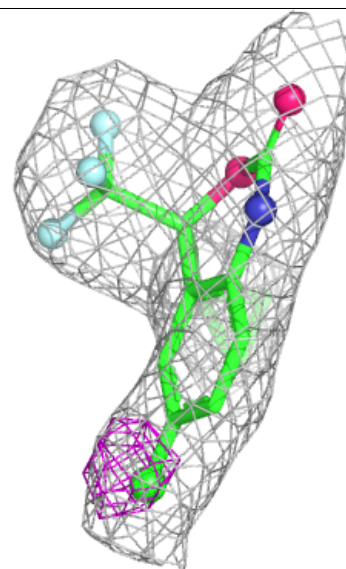
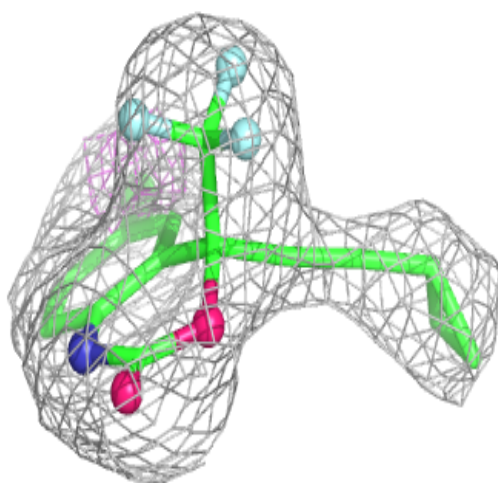
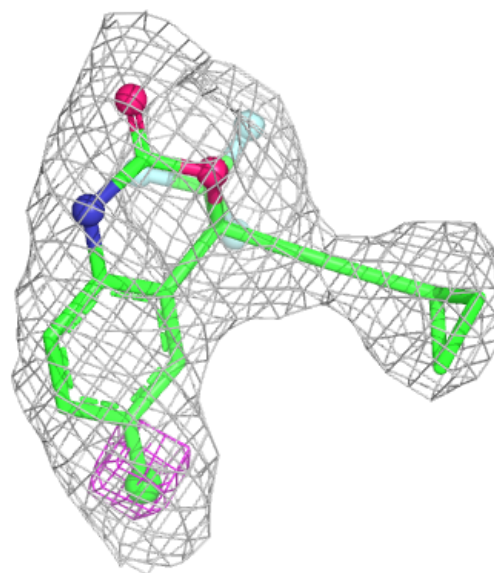
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EFZ	A	2000	21/21	0.95	0.08	31,34,36,36	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 2000:

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 [i](#)

There are no such residues in this entry.