



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:58 PM GMT

PDB ID : 1IKW  
Title : Wild Type 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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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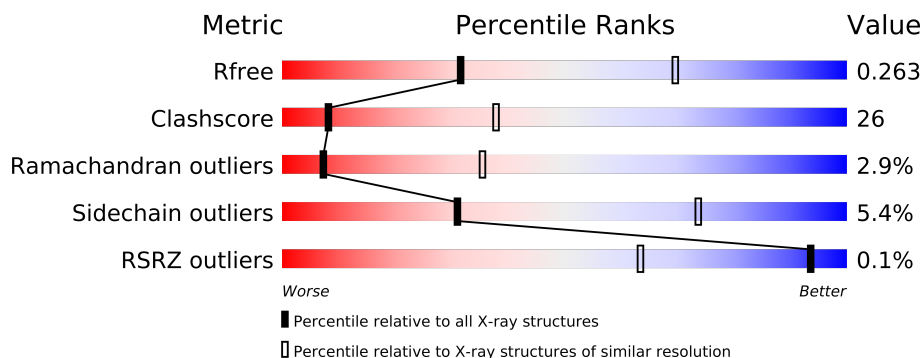
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	427	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7890 atoms, of which 0 are hydrogen and 0 are deuterium.

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	557	Total	C	N	O	S	2	0	0
			4523	2927	754	834	8			

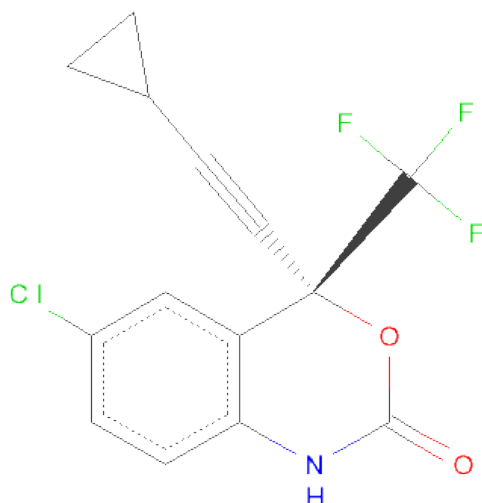
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	478	GLN	GLU	ENGINEERED	UNP P03366

- Molecule 2 is a protein called POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	30	0	0
			3346	2180	550	610	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<sub>14</sub>H<sub>9</sub>ClF<sub>3</sub>NO<sub>2</sub>).



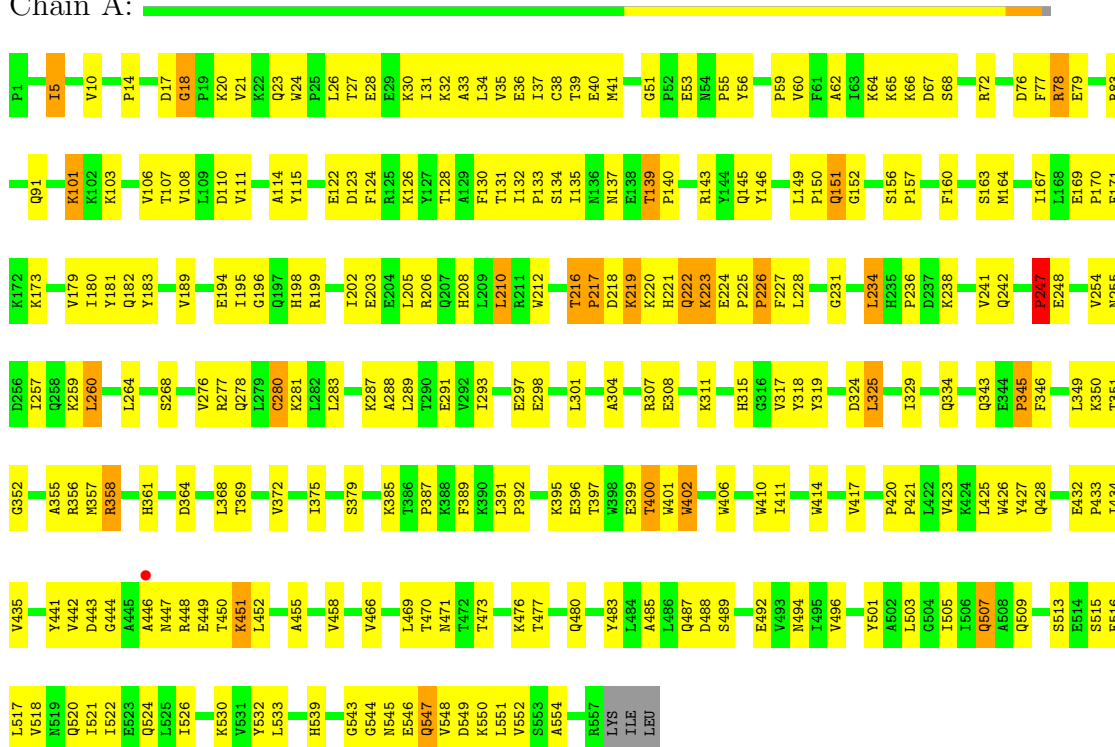
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
3	A	1	21	14	1	3	1	2	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: POL POLYPROTEIN

Chain A:



#### • Molecule 2: POL POLYPROTEIN

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.55Å 157.31Å 157.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.69 – 3.00 24.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.69-3.00) 99.4 (24.68-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.218 , 0.272 0.218 , 0.263	Depositor DCC
$R_{free}$ test set	1830 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.1	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36519 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.42	0/4641	0.64	0/6305
2	B	0.40	0/3440	0.64	0/4674
All	All	0.41	0/8081	0.64	0/10979

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4523	0	4579	252	1
2	B	3346	0	3379	180	0
3	A	21	0	8	1	0
All	All	7890	0	7966	418	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (418) close contacts within the same asymmetric unit are listed below.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.36	1.04
1:A:223:LYS:HG3	1:A:224:GLU:H	1.29	0.97
2:B:1283:LEU:HD13	2:B:1293:ILE:HG13	1.47	0.94
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.49	0.94
1:A:65:LYS:HG3	1:A:66:LYS:H	1.33	0.94
1:A:219:LYS:HD3	1:A:220:LYS:HE2	1.53	0.91
1:A:543:GLY:H	2:B:1284:ARG:HD2	1.38	0.89
2:B:1263:LYS:HE2	2:B:1425:LEU:HA	1.53	0.88
1:A:458:VAL:HG21	1:A:547:GLN:HE22	1.38	0.87
2:B:1275:LYS:HE3	2:B:1277:ARG:HB3	1.56	0.86
2:B:1215:THR:HG22	2:B:1216:THR:H	1.41	0.84
1:A:228:LEU:HB3	1:A:242:GLN:HE22	1.43	0.83
2:B:1184:MET:O	2:B:1185:ASP:HB2	1.79	0.81
1:A:450:THR:O	1:A:451:LYS:HB2	1.81	0.81
1:A:225:PRO:HA	1:A:226:PRO:O	1.80	0.80
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.63	0.79
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.63	0.79
1:A:107:THR:HB	1:A:223:LYS:HB3	1.65	0.78
2:B:1169:GLU:HB3	2:B:1170:PRO:HD3	1.67	0.77
1:A:435:VAL:HG13	2:B:1290:THR:HG21	1.68	0.76
1:A:458:VAL:CG2	1:A:547:GLN:HE22	1.99	0.75
1:A:106:VAL:HG13	1:A:225:PRO:HG2	1.66	0.75
1:A:223:LYS:CG	1:A:224:GLU:H	1.93	0.75
1:A:26:LEU:HD23	1:A:133:PRO:HG2	1.69	0.75
1:A:450:THR:HG22	1:A:452:LEU:HG	1.68	0.74
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.02	0.74
1:A:396:GLU:O	1:A:400:THR:HG22	1.87	0.74
2:B:1417:VAL:HG22	2:B:1418:ASN:H	1.53	0.73
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.54	0.73
1:A:64:LYS:HD3	1:A:68:SER:HB3	1.69	0.72
2:B:1059:PRO:HG2	2:B:1076:ASP:HB3	1.71	0.72
1:A:32:LYS:O	1:A:36:GLU:HG3	1.90	0.71
2:B:1395:LYS:O	2:B:1399:GLU:HG3	1.89	0.71
1:A:223:LYS:HG3	1:A:224:GLU:N	2.05	0.71
2:B:1090:VAL:HG23	2:B:1091:GLN:N	2.05	0.71
2:B:1246:LEU:HD12	2:B:1307:ARG:HB3	1.73	0.70
2:B:1254:VAL:HG23	2:B:1291:GLU:O	1.91	0.70
1:A:23:GLN:HG2	1:A:133:PRO:HG3	1.72	0.70
1:A:101:LYS:N	1:A:101:LYS:HE3	2.06	0.70
2:B:1287:LYS:HD3	2:B:1291:GLU:OE2	1.92	0.69
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.73	0.69
1:A:473:THR:O	1:A:477:THR:HG23	1.93	0.69
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.20	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:458:VAL:HG21	1:A:547:GLN:NE2	2.08	0.68
2:B:1050:ILE:CG2	2:B:1145:GLN:HG2	2.23	0.68
1:A:543:GLY:N	2:B:1284:ARG:HD2	2.06	0.68
1:A:447:ASN:OD1	1:A:449:GLU:HG2	1.93	0.68
2:B:1122:GLU:H	2:B:1122:GLU:CD	1.96	0.68
1:A:131:THR:CG2	1:A:143:ARG:HG2	2.22	0.68
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.59	0.67
2:B:1393:ILE:HG12	2:B:1394:GLN:N	2.09	0.67
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.77	0.67
2:B:1231:GLY:O	2:B:1232:TYR:HB3	1.96	0.66
1:A:31:ILE:O	1:A:35:VAL:HG23	1.95	0.66
1:A:441:TYR:CE2	1:A:544:GLY:HA3	2.31	0.66
2:B:1007:THR:HG22	2:B:1119:PRO:HG2	1.77	0.66
2:B:1305:GLU:O	2:B:1309:ILE:HG13	1.96	0.65
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.78	0.65
2:B:1296:THR:HG22	2:B:1298:GLU:H	1.62	0.65
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.61	0.65
1:A:151:GLN:HE21	1:A:151:GLN:C	2.00	0.65
1:A:180:ILE:HG12	1:A:189:VAL:HG22	1.79	0.64
2:B:1157:PRO:HG2	2:B:1184:MET:HA	1.79	0.64
2:B:1216:THR:HB	2:B:1217:PRO:HD2	1.78	0.64
2:B:1154:LYS:HE2	2:B:1184:MET:CE	2.27	0.64
2:B:1314:VAL:HB	2:B:1317:VAL:HG21	1.78	0.64
2:B:1282:LEU:HD11	2:B:1296:THR:OG1	1.97	0.64
2:B:1293:ILE:H	2:B:1293:ILE:HD13	1.63	0.63
2:B:1257:ILE:O	2:B:1261:VAL:HG23	1.98	0.63
2:B:1283:LEU:HD22	2:B:1293:ILE:HB	1.80	0.63
2:B:1084:THR:HG22	2:B:1087:PHE:HB3	1.79	0.63
1:A:64:LYS:HB3	1:A:68:SER:HA	1.80	0.63
1:A:64:LYS:HD3	1:A:68:SER:CB	2.28	0.62
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.33	0.62
2:B:1324:ASP:O	2:B:1343:GLN:HG2	2.00	0.62
2:B:1393:ILE:HG12	2:B:1394:GLN:H	1.64	0.62
2:B:1267:ALA:HB1	2:B:1310:LEU:HD21	1.81	0.62
1:A:361:HIS:HD2	1:A:513:SER:OG	1.83	0.62
2:B:1296:THR:HB	2:B:1299:ALA:HB2	1.81	0.61
1:A:441:TYR:O	1:A:548:VAL:HG21	1.99	0.61
2:B:1253:THR:O	2:B:1257:ILE:HG22	2.00	0.61
1:A:128:THR:OG1	1:A:146:TYR:HB2	2.00	0.61
1:A:458:VAL:HG23	1:A:548:VAL:HG13	1.83	0.61
2:B:1024:TRP:CD2	2:B:1025:PRO:HD2	2.35	0.61
1:A:218:ASP:HB3	1:A:219:LYS:CE	2.31	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:351:THR:HG22	1:A:352:GLY:N	2.16	0.61
2:B:1154:LYS:HE2	2:B:1184:MET:HE1	1.82	0.60
1:A:101:LYS:HE3	1:A:101:LYS:H	1.64	0.60
2:B:1275:LYS:N	2:B:1306:ASN:HD21	2.00	0.60
1:A:26:LEU:CD2	1:A:133:PRO:HG2	2.30	0.60
1:A:458:VAL:CB	1:A:548:VAL:HG22	2.32	0.60
2:B:1086:ASP:O	2:B:1090:VAL:HG22	2.02	0.60
1:A:115:TYR:HD1	1:A:151:GLN:HA	1.66	0.60
2:B:1278:GLN:HB3	2:B:1298:GLU:HG3	1.82	0.60
2:B:1216:THR:HB	2:B:1217:PRO:CD	2.31	0.59
2:B:1156:SER:HB2	2:B:1157:PRO:HD3	1.84	0.59
1:A:107:THR:CB	1:A:223:LYS:HB3	2.32	0.59
2:B:1168:LEU:HD13	2:B:1180:ILE:HG21	1.83	0.59
1:A:53:GLU:O	1:A:55:PRO:HD3	2.03	0.59
1:A:361:HIS:CD2	1:A:513:SER:OG	2.56	0.59
1:A:372:VAL:HG11	1:A:411:ILE:HG13	1.84	0.59
1:A:221:HIS:C	1:A:223:LYS:H	2.05	0.59
2:B:1090:VAL:CG2	2:B:1091:GLN:N	2.65	0.59
2:B:1091:GLN:O	2:B:1092:LEU:HD23	2.03	0.59
2:B:1353:LYS:HB3	2:B:1353:LYS:NZ	2.18	0.59
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.36	0.58
2:B:1203:GLU:HA	2:B:1206:ARG:HD3	1.86	0.58
2:B:1266:TRP:C	2:B:1268:SER:H	2.05	0.58
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.85	0.58
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.86	0.58
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.86	0.58
2:B:1254:VAL:HG12	2:B:1258:GLN:HE21	1.68	0.58
1:A:219:LYS:HD2	1:A:220:LYS:HG2	1.86	0.58
2:B:1114:ALA:HB2	2:B:1214:LEU:HD22	1.86	0.58
2:B:1031:ILE:O	2:B:1035:VAL:HG13	2.02	0.58
1:A:231:GLY:C	1:A:242:GLN:HG2	2.24	0.57
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.39	0.57
1:A:139:THR:HG22	1:A:140:PRO:CD	2.24	0.57
1:A:547:GLN:NE2	1:A:548:VAL:N	2.52	0.57
1:A:485:ALA:O	1:A:489:SER:CB	2.53	0.57
1:A:219:LYS:HD2	1:A:219:LYS:H	1.70	0.57
1:A:218:ASP:HB3	1:A:219:LYS:HE2	1.87	0.57
1:A:33:ALA:O	1:A:37:ILE:HG13	2.05	0.57
2:B:1283:LEU:HD13	2:B:1293:ILE:CG1	2.27	0.56
1:A:103:LYS:HE3	1:A:179:VAL:HG11	1.87	0.56
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.86	0.56
2:B:1365:VAL:O	2:B:1369:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1379:SER:OG	2:B:1387:PRO:HD3	2.05	0.56
1:A:28:GLU:HG2	1:A:135:ILE:HG23	1.87	0.56
1:A:223:LYS:CG	1:A:224:GLU:N	2.67	0.56
2:B:1293:ILE:N	2:B:1293:ILE:HD13	2.19	0.56
2:B:1422:LEU:HD23	2:B:1422:LEU:C	2.26	0.56
2:B:1280:CYS:C	2:B:1282:LEU:H	2.09	0.56
1:A:317:VAL:HG22	1:A:318:TYR:N	2.20	0.56
1:A:458:VAL:CB	1:A:547:GLN:HE22	2.18	0.56
1:A:106:VAL:HG13	1:A:225:PRO:CG	2.36	0.56
2:B:1019:PRO:HG2	2:B:1080:LEU:HB2	1.88	0.56
2:B:1060:VAL:HG12	2:B:1075:VAL:HG22	1.87	0.56
2:B:1028:GLU:HB2	2:B:1135:ILE:HD11	1.88	0.56
1:A:426:TRP:O	1:A:427:TYR:HB3	2.06	0.56
2:B:1076:ASP:OD1	2:B:1078:ARG:HB2	2.07	0.55
1:A:27:THR:O	1:A:31:ILE:HG13	2.06	0.55
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.88	0.55
1:A:548:VAL:O	1:A:552:VAL:HG23	2.05	0.55
2:B:1320:ASP:OD2	2:B:1323:LYS:HG3	2.06	0.55
1:A:103:LYS:HE3	1:A:179:VAL:CG1	2.36	0.55
1:A:17:ASP:O	1:A:83:ARG:NH1	2.39	0.55
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.88	0.55
2:B:1193:LEU:HD23	2:B:1197:GLN:HB3	1.89	0.55
1:A:301:LEU:O	1:A:304:ALA:HB3	2.07	0.55
1:A:351:THR:CG2	1:A:352:GLY:N	2.70	0.55
1:A:435:VAL:HG22	2:B:1290:THR:CG2	2.38	0.54
2:B:1084:THR:HG22	2:B:1084:THR:O	2.06	0.54
2:B:1073:LYS:NZ	2:B:1130:PHE:CZ	2.72	0.54
2:B:1271:TYR:O	2:B:1274:ILE:HG12	2.06	0.54
1:A:503:LEU:O	1:A:507:GLN:HB2	2.07	0.54
1:A:543:GLY:HA2	2:B:1285:GLY:H	1.72	0.54
1:A:131:THR:CG2	1:A:143:ARG:NH1	2.70	0.54
2:B:1090:VAL:CG2	2:B:1091:GLN:H	2.20	0.54
1:A:450:THR:CG2	1:A:452:LEU:HG	2.37	0.54
2:B:1278:GLN:HB3	2:B:1298:GLU:CD	2.27	0.54
2:B:1296:THR:HG21	2:B:1298:GLU:OE2	2.07	0.54
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.42	0.54
2:B:1260:LEU:HD22	2:B:1279:LEU:HD21	1.90	0.54
1:A:37:ILE:O	1:A:40:GLU:HB3	2.07	0.54
1:A:65:LYS:HG3	1:A:66:LYS:N	2.12	0.54
2:B:1023:GLN:OE1	2:B:1059:PRO:HA	2.08	0.54
1:A:62:ALA:HA	1:A:72:ARG:O	2.07	0.53
2:B:1257:ILE:O	2:B:1257:ILE:HD12	2.07	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:225:PRO:HA	1:A:226:PRO:C	2.29	0.53
2:B:1215:THR:HG22	2:B:1216:THR:N	2.19	0.53
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.90	0.53
2:B:1266:TRP:HB3	2:B:1427:TYR:OH	2.07	0.53
1:A:458:VAL:CG2	1:A:548:VAL:HG22	2.39	0.53
1:A:106:VAL:HG22	1:A:227:PHE:HE2	1.74	0.53
1:A:20:LYS:HG2	1:A:55:PRO:O	2.08	0.53
1:A:402:TRP:CD1	1:A:402:TRP:C	2.81	0.53
1:A:108:VAL:O	1:A:221:HIS:O	2.27	0.52
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.44	0.52
2:B:1024:TRP:CG	2:B:1025:PRO:HD2	2.44	0.52
2:B:1252:TRP:CE3	2:B:1252:TRP:HA	2.42	0.52
2:B:1266:TRP:O	2:B:1268:SER:N	2.40	0.52
2:B:1037:ILE:O	2:B:1041:MET:HG3	2.10	0.52
1:A:308:GLU:O	1:A:311:LYS:HG2	2.09	0.52
1:A:203:GLU:OE2	1:A:206:ARG:HD3	2.10	0.52
1:A:466:VAL:CG2	1:A:551:LEU:HD13	2.40	0.52
2:B:1278:GLN:HB3	2:B:1298:GLU:CG	2.40	0.52
1:A:473:THR:HG23	1:A:476:LYS:NZ	2.25	0.52
2:B:1286:THR:HG22	2:B:1286:THR:O	2.10	0.52
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.91	0.52
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.25	0.51
2:B:1366:LYS:O	2:B:1370:GLU:HG3	2.11	0.51
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.44	0.51
2:B:1393:ILE:CG1	2:B:1394:GLN:H	2.22	0.51
2:B:1420:PRO:C	2:B:1422:LEU:H	2.14	0.51
2:B:1393:ILE:CG1	2:B:1394:GLN:N	2.74	0.51
2:B:1241:VAL:O	2:B:1243:PRO:HD3	2.11	0.51
2:B:1066:LYS:O	2:B:1067:ASP:HB2	2.09	0.51
2:B:1317:VAL:HG12	2:B:1347:LYS:HB3	1.93	0.51
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.46	0.51
2:B:1280:CYS:O	2:B:1281:LYS:HB3	2.11	0.51
1:A:485:ALA:O	1:A:489:SER:HB2	2.10	0.51
1:A:410:TRP:CG	1:A:411:ILE:N	2.79	0.51
2:B:1085:GLN:HA	2:B:1088:TRP:CE2	2.46	0.50
1:A:428:GLN:HA	1:A:509:GLN:NE2	2.26	0.50
1:A:20:LYS:HZ1	1:A:55:PRO:HB2	1.74	0.50
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.94	0.50
1:A:218:ASP:HB3	1:A:219:LYS:HE3	1.92	0.50
1:A:247:PRO:O	1:A:248:GLU:HB3	2.12	0.50
2:B:1274:ILE:HA	2:B:1306:ASN:ND2	2.26	0.50
1:A:151:GLN:CA	1:A:151:GLN:HE21	2.24	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1254:VAL:CG1	2:B:1258:GLN:HE21	2.25	0.50
2:B:1154:LYS:HG2	2:B:1184:MET:HE2	1.93	0.50
1:A:206:ARG:CZ	1:A:217:PRO:O	2.60	0.50
2:B:1153:TRP:CE2	2:B:1155:GLY:HA3	2.46	0.50
1:A:543:GLY:CA	2:B:1284:ARG:HB3	2.42	0.49
2:B:1283:LEU:CD1	2:B:1293:ILE:HG13	2.32	0.49
1:A:406:TRP:CZ2	2:B:1418:ASN:OD1	2.64	0.49
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.42	0.49
1:A:221:HIS:O	1:A:223:LYS:N	2.45	0.49
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.12	0.49
1:A:410:TRP:HA	1:A:410:TRP:HE3	1.78	0.49
1:A:346:PHE:N	1:A:346:PHE:CD2	2.76	0.49
1:A:401:TRP:HB2	1:A:425:LEU:HD11	1.94	0.49
1:A:526:ILE:O	1:A:526:ILE:HG22	2.12	0.49
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.47	0.49
2:B:1279:LEU:HB2	2:B:1302:GLU:OE1	2.13	0.49
2:B:1402:TRP:C	2:B:1404:GLU:H	2.16	0.49
2:B:1168:LEU:CD1	2:B:1180:ILE:HG21	2.42	0.49
2:B:1270:ILE:O	2:B:1271:TYR:HB2	2.12	0.49
2:B:1183:TYR:CE2	2:B:1184:MET:HE3	2.47	0.49
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.48	0.49
1:A:543:GLY:CA	2:B:1284:ARG:HD2	2.43	0.48
2:B:1417:VAL:HG22	2:B:1418:ASN:N	2.24	0.48
1:A:111:VAL:HG21	1:A:164:MET:CE	2.43	0.48
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.48	0.48
1:A:443:ASP:HB3	1:A:552:VAL:HG21	1.95	0.48
1:A:38:CYS:O	1:A:39:THR:C	2.52	0.48
1:A:516:GLU:O	1:A:520:GLN:HG3	2.13	0.48
2:B:1084:THR:CG2	2:B:1087:PHE:HB3	2.42	0.48
2:B:1422:LEU:O	2:B:1425:LEU:HG	2.13	0.48
2:B:1154:LYS:HE2	2:B:1184:MET:HE2	1.96	0.48
2:B:1369:THR:HG22	2:B:1398:TRP:CH2	2.49	0.48
2:B:1153:TRP:CZ2	2:B:1155:GLY:HA3	2.49	0.48
1:A:470:THR:O	1:A:471:ASN:HB2	2.13	0.48
1:A:417:VAL:O	1:A:417:VAL:HG13	2.14	0.48
2:B:1252:TRP:HE3	2:B:1252:TRP:HA	1.79	0.47
2:B:1017:ASP:O	2:B:1083:ARG:NH1	2.47	0.47
1:A:494:ASN:HB3	2:B:1289:LEU:HD12	1.96	0.47
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.95	0.47
1:A:134:SER:HB2	1:A:139:THR:OG1	2.14	0.47
2:B:1090:VAL:HG23	2:B:1091:GLN:H	1.73	0.47
2:B:1050:ILE:HG23	2:B:1145:GLN:HG2	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:411:ILE:HG23	1:A:411:ILE:O	2.15	0.47
1:A:375:ILE:O	1:A:379:SER:HB2	2.14	0.47
1:A:522:ILE:O	1:A:526:ILE:HG13	2.14	0.47
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.96	0.47
2:B:1115:TYR:HB3	2:B:1149:LEU:HB2	1.96	0.47
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.97	0.47
1:A:276:VAL:O	1:A:280:CYS:HB2	2.15	0.47
1:A:458:VAL:HG11	1:A:547:GLN:NE2	2.30	0.47
1:A:108:VAL:HB	1:A:227:PHE:CE1	2.50	0.46
1:A:307:ARG:HG3	1:A:307:ARG:NH1	2.28	0.46
1:A:115:TYR:O	1:A:149:LEU:HB2	2.15	0.46
1:A:206:ARG:HE	1:A:216:THR:HG23	1.80	0.46
1:A:455:ALA:CB	1:A:469:LEU:HD11	2.45	0.46
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.97	0.46
2:B:1413:GLU:OE1	2:B:1413:GLU:HA	2.15	0.46
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.56	0.46
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.50	0.46
2:B:1353:LYS:HG2	2:B:1354:TYR:N	2.31	0.46
1:A:254:VAL:HG22	1:A:293:ILE:CD1	2.45	0.46
2:B:1252:TRP:O	2:B:1292:VAL:HG23	2.16	0.46
2:B:1395:LYS:HG3	2:B:1416:PHE:CE2	2.50	0.46
1:A:110:ASP:OD1	1:A:217:PRO:HG2	2.16	0.46
1:A:221:HIS:C	1:A:223:LYS:N	2.69	0.46
1:A:195:ILE:HG12	1:A:199:ARG:CZ	2.46	0.46
1:A:107:THR:HG23	1:A:198:HIS:NE2	2.31	0.45
2:B:1283:LEU:O	2:B:1284:ARG:HD3	2.16	0.45
2:B:1314:VAL:HB	2:B:1317:VAL:CG2	2.45	0.45
1:A:355:ALA:O	1:A:356:ARG:C	2.54	0.45
1:A:356:ARG:NH1	1:A:358:ARG:HA	2.31	0.45
2:B:1280:CYS:C	2:B:1282:LEU:N	2.70	0.45
1:A:434:ILE:HG13	1:A:494:ASN:OD1	2.17	0.45
1:A:548:VAL:HG12	1:A:552:VAL:CG2	2.45	0.45
2:B:1264:LEU:CD1	2:B:1279:LEU:HD23	2.47	0.45
2:B:1283:LEU:CD2	2:B:1293:ILE:HB	2.47	0.45
1:A:550:LYS:O	1:A:554:ALA:HB2	2.16	0.45
1:A:545:ASN:O	1:A:549:ASP:HB2	2.17	0.45
1:A:202:ILE:O	1:A:205:LEU:HB3	2.17	0.45
1:A:228:LEU:CB	1:A:242:GLN:HE22	2.22	0.45
1:A:287:LYS:HB3	1:A:291:GLU:OE2	2.16	0.45
1:A:151:GLN:HE21	1:A:152:GLY:N	2.14	0.45
2:B:1241:VAL:HG12	2:B:1242:GLN:N	2.32	0.45
2:B:1426:TRP:HA	2:B:1426:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:THR:HA	1:A:223:LYS:CB	2.47	0.45
1:A:236:PRO:HA	3:A:2000:EFZ:H3	1.99	0.45
1:A:108:VAL:CG1	1:A:227:PHE:HE1	2.30	0.44
1:A:260:LEU:HD22	1:A:264:LEU:HD11	1.98	0.44
2:B:1249:LYS:HB3	2:B:1252:TRP:CZ3	2.52	0.44
2:B:1267:ALA:O	2:B:1274:ILE:HG13	2.17	0.44
2:B:1274:ILE:HG23	2:B:1306:ASN:CG	2.37	0.44
2:B:1306:ASN:HA	2:B:1306:ASN:HD22	1.59	0.44
2:B:1296:THR:CG2	2:B:1298:GLU:HG2	2.47	0.44
1:A:368:LEU:O	1:A:372:VAL:HG23	2.17	0.44
1:A:173:LYS:HD3	1:A:173:LYS:C	2.38	0.44
1:A:543:GLY:HA3	2:B:1284:ARG:HD2	1.98	0.44
2:B:1422:LEU:HD21	2:B:1427:TYR:OXT	2.18	0.44
2:B:1312:GLU:HB3	2:B:1313:PRO:HD2	1.98	0.44
1:A:195:ILE:CD1	1:A:199:ARG:NH2	2.81	0.44
1:A:151:GLN:NE2	1:A:151:GLN:CA	2.81	0.44
1:A:455:ALA:HB3	1:A:469:LEU:HD11	2.00	0.44
1:A:5:ILE:HD12	1:A:167:ILE:HG13	1.99	0.44
2:B:1330:GLN:NE2	2:B:1338:THR:OG1	2.49	0.44
2:B:1206:ARG:HG2	2:B:1216:THR:HG21	1.99	0.44
1:A:268:SER:O	1:A:351:THR:HG22	2.18	0.44
1:A:329:ILE:O	1:A:392:PRO:HD3	2.18	0.44
2:B:1028:GLU:CB	2:B:1135:ILE:HD11	2.48	0.44
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.18	0.44
1:A:223:LYS:O	1:A:224:GLU:C	2.57	0.44
1:A:30:LYS:O	1:A:33:ALA:HB3	2.18	0.44
2:B:1260:LEU:HD23	2:B:1260:LEU:O	2.18	0.44
1:A:210:LEU:C	1:A:212:TRP:H	2.21	0.44
1:A:483:TYR:O	1:A:487:GLN:HG3	2.17	0.44
1:A:521:ILE:HG22	1:A:521:ILE:O	2.17	0.44
1:A:65:LYS:NZ	1:A:72:ARG:HH11	2.16	0.43
1:A:77:PHE:O	1:A:79:GLU:N	2.51	0.43
1:A:5:ILE:HD13	1:A:163:SER:HB3	1.99	0.43
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.54	0.43
1:A:131:THR:HG22	1:A:143:ARG:CG	2.36	0.43
1:A:435:VAL:HG22	2:B:1290:THR:HG23	1.99	0.43
1:A:67:ASP:O	1:A:68:SER:HB2	2.18	0.43
1:A:210:LEU:C	1:A:212:TRP:N	2.71	0.43
2:B:1195:ILE:HG23	2:B:1196:GLY:N	2.32	0.43
1:A:361:HIS:CD2	1:A:361:HIS:N	2.87	0.43
1:A:234:LEU:HD13	1:A:234:LEU:N	2.34	0.43
1:A:122:GLU:O	1:A:124:PHE:N	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:544:GLY:O	1:A:548:VAL:HG23	2.18	0.43
1:A:473:THR:HG23	1:A:476:LYS:HZ2	1.83	0.43
1:A:156:SER:N	1:A:157:PRO:CD	2.82	0.43
2:B:1402:TRP:CE2	2:B:1403:THR:CG2	3.02	0.43
1:A:492:GLU:HA	1:A:530:LYS:O	2.18	0.43
1:A:131:THR:HG21	1:A:143:ARG:NH1	2.33	0.43
2:B:1414:TRP:O	2:B:1414:TRP:HD1	2.01	0.43
2:B:1292:VAL:HG22	2:B:1293:ILE:N	2.33	0.43
1:A:53:GLU:CD	1:A:53:GLU:H	2.21	0.43
1:A:496:VAL:CG2	2:B:1289:LEU:HD11	2.49	0.43
2:B:1207:GLN:O	2:B:1211:ARG:HD3	2.18	0.43
1:A:476:LYS:O	1:A:480:GLN:N	2.47	0.43
1:A:304:ALA:O	1:A:307:ARG:HB2	2.19	0.43
1:A:231:GLY:O	1:A:242:GLN:HG2	2.19	0.42
2:B:1195:ILE:CG2	2:B:1196:GLY:N	2.82	0.42
2:B:1249:LYS:HB2	2:B:1249:LYS:HE3	1.81	0.42
2:B:1274:ILE:HG23	2:B:1306:ASN:ND2	2.33	0.42
2:B:1231:GLY:O	2:B:1232:TYR:CB	2.66	0.42
2:B:1296:THR:O	2:B:1299:ALA:HB3	2.18	0.42
1:A:277:ARG:NH1	1:A:281:LYS:HD2	2.33	0.42
1:A:65:LYS:HZ3	1:A:72:ARG:HH11	1.66	0.42
2:B:1425:LEU:HD23	2:B:1425:LEU:N	2.34	0.42
1:A:410:TRP:O	1:A:411:ILE:HB	2.18	0.42
2:B:1419:THR:HA	2:B:1420:PRO:HD3	1.67	0.42
2:B:1278:GLN:HB2	2:B:1302:GLU:CD	2.40	0.42
1:A:135:ILE:HG13	1:A:135:ILE:H	1.58	0.42
1:A:324:ASP:O	1:A:343:GLN:HG2	2.19	0.42
2:B:1038:CYS:SG	2:B:1132:ILE:HD11	2.60	0.42
1:A:515:SER:HB3	1:A:518:VAL:HB	2.01	0.42
1:A:546:GLU:O	1:A:549:ASP:HB3	2.19	0.42
1:A:397:THR:O	1:A:400:THR:HG23	2.19	0.42
1:A:357:MET:O	1:A:358:ARG:HB3	2.19	0.42
1:A:222:GLN:O	1:A:223:LYS:C	2.58	0.42
1:A:543:GLY:HA2	2:B:1284:ARG:HB3	2.00	0.42
1:A:351:THR:CG2	1:A:352:GLY:H	2.32	0.42
1:A:131:THR:O	1:A:133:PRO:HD3	2.20	0.42
1:A:101:LYS:CE	1:A:101:LYS:N	2.81	0.42
1:A:77:PHE:O	1:A:78:ARG:C	2.58	0.42
2:B:1298:GLU:HG2	2:B:1299:ALA:N	2.35	0.41
1:A:208:HIS:O	1:A:212:TRP:HD1	2.03	0.41
2:B:1414:TRP:O	2:B:1414:TRP:CD1	2.73	0.41
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:LEU:HD22	1:A:26:LEU:N	2.35	0.41
2:B:1422:LEU:O	2:B:1422:LEU:HD23	2.21	0.41
2:B:1402:TRP:CE2	2:B:1403:THR:HG23	2.54	0.41
1:A:194:GLU:O	1:A:196:GLY:N	2.54	0.41
2:B:1046:LYS:HE2	2:B:1116:PHE:HB3	2.01	0.41
2:B:1064:LYS:O	2:B:1065:LYS:O	2.38	0.41
2:B:1283:LEU:HD21	2:B:1294:PRO:HD2	2.02	0.41
2:B:1244:ILE:HD13	2:B:1427:TYR:CE2	2.55	0.41
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.55	0.41
1:A:108:VAL:HB	1:A:227:PHE:CZ	2.55	0.41
2:B:1344:GLU:O	2:B:1347:LYS:HB2	2.20	0.41
1:A:443:ASP:OD1	1:A:444:GLY:N	2.49	0.41
1:A:455:ALA:H	1:A:469:LEU:CD1	2.34	0.41
2:B:1266:TRP:CE3	2:B:1425:LEU:HD21	2.56	0.41
1:A:550:LYS:HA	1:A:550:LYS:HD2	1.82	0.41
2:B:1072:ARG:HG3	2:B:1072:ARG:HH11	1.85	0.41
1:A:543:GLY:CA	2:B:1285:GLY:H	2.34	0.41
1:A:450:THR:HG21	1:A:452:LEU:HD12	2.03	0.41
2:B:1296:THR:HG21	2:B:1298:GLU:HG2	2.01	0.41
1:A:317:VAL:CG2	1:A:318:TYR:N	2.84	0.41
2:B:1005:ILE:HD11	2:B:1118:VAL:HG13	2.02	0.41
1:A:420:PRO:HA	1:A:421:PRO:C	2.41	0.41
2:B:1129:ALA:HA	2:B:1144:TYR:O	2.21	0.41
2:B:1333:GLY:O	2:B:1334:GLN:HB2	2.21	0.41
2:B:1105:SER:O	2:B:1190:GLY:HA2	2.21	0.41
2:B:1120:LEU:O	2:B:1121:ASP:C	2.59	0.41
1:A:91:GLN:HE22	1:A:183:TYR:HD1	1.66	0.41
2:B:1266:TRP:C	2:B:1268:SER:N	2.71	0.40
2:B:1427:TYR:O	2:B:1427:TYR:CD1	2.74	0.40
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.36	0.40
2:B:1326:ILE:O	2:B:1341:ILE:HA	2.21	0.40
1:A:24:TRP:O	1:A:26:LEU:HD22	2.22	0.40
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.95	0.40
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.40	0.40
1:A:51:GLY:HA3	1:A:53:GLU:OE1	2.22	0.40
1:A:350:LYS:HG2	1:A:351:THR:N	2.35	0.40
1:A:379:SER:OG	1:A:387:PRO:HD3	2.20	0.40
1:A:434:ILE:HD13	1:A:530:LYS:HB3	2.04	0.40
2:B:1371:ALA:O	2:B:1375:ILE:HG13	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:448:ARG:NH2	1:A:448:ARG:NH2[3.557]	1.73	0.47

## 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	555/560 (99%)	471 (85%)	68 (12%)	16 (3%)	7	35
2	B	399/427 (93%)	344 (86%)	43 (11%)	12 (3%)	7	34
All	All	954/987 (97%)	815 (85%)	111 (12%)	28 (3%)	7	35

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	223	LYS
2	B	1065	LYS
2	B	1267	ALA
2	B	1294	PRO
1	A	76	ASP
1	A	137	ASN
1	A	451	LYS
1	A	539	HIS
2	B	1252	TRP
1	A	14	PRO
1	A	78	ARG
1	A	345	PRO
1	A	358	ARG
2	B	1184	MET
1	A	18	GLY
1	A	123	ASP
1	A	226	PRO
2	B	1232	TYR
2	B	1345	PRO
1	A	217	PRO
1	A	222	GLN
1	A	247	PRO

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Mol	Chain	Res	Type
2	B	1085	GLN
2	B	1185	ASP
2	B	1403	THR
2	B	1321	PRO
2	B	1018	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	495/500 (99%)	466 (94%)	29 (6%)	28	70
2	B	369/389 (95%)	351 (95%)	18 (5%)	35	78
All	All	864/889 (97%)	817 (95%)	47 (5%)	31	74

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

Mol	Chain	Res	Type
1	A	10	VAL
1	A	101	LYS
1	A	126	LYS
1	A	139	THR
1	A	145	GLN
1	A	151	GLN
1	A	182	GLN
1	A	210	LEU
1	A	216	THR
1	A	219	LYS
1	A	234	LEU
1	A	241	VAL
1	A	247	PRO
1	A	259	LYS
1	A	260	LEU
1	A	280	CYS
1	A	297	GLU
1	A	325	LEU
1	A	334	GLN
1	A	345	PRO

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Mol	Chain	Res	Type
1	A	369	THR
1	A	400	THR
1	A	402	TRP
1	A	432	GLU
1	A	488	ASP
1	A	507	GLN
1	A	517	LEU
1	A	533	LEU
1	A	547	GLN
2	B	1039	THR
2	B	1072	ARG
2	B	1078	ARG
2	B	1086	ASP
2	B	1139	THR
2	B	1185	ASP
2	B	1252	TRP
2	B	1257	ILE
2	B	1266	TRP
2	B	1293	ILE
2	B	1306	ASN
2	B	1330	GLN
2	B	1345	PRO
2	B	1356	ARG
2	B	1418	ASN
2	B	1422	LEU
2	B	1425	LEU
2	B	1426	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	145	GLN
1	A	151	GLN
1	A	182	GLN
1	A	208	HIS
1	A	242	GLN
1	A	278	GLN
1	A	332	GLN
1	A	336	GLN
1	A	361	HIS
1	A	407	GLN

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Mol	Chain	Res	Type
1	A	428	GLN
1	A	509	GLN
1	A	524	GLN
1	A	547	GLN
2	B	1137	ASN
2	B	1161	GLN
2	B	1182	GLN
2	B	1258	GLN
2	B	1306	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	4.32	12 (52%)	36,36,36	2.11	12 (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
3	EFZ	A	2000	-	-	2/14/32/32	0/0/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	EFZ	C4-CL	-16.80	1.35	1.74
3	A	2000	EFZ	C7-C6	5.35	1.58	1.51
3	A	2000	EFZ	C9-C8	5.29	1.34	1.19
3	A	2000	EFZ	C14-N	3.91	1.42	1.35
3	A	2000	EFZ	C5-C6	3.37	1.45	1.39
3	A	2000	EFZ	C1-C6	3.33	1.44	1.40
3	A	2000	EFZ	C3-C4	2.94	1.43	1.38
3	A	2000	EFZ	C5-C4	2.80	1.43	1.38
3	A	2000	EFZ	C3-C2	2.72	1.44	1.38
3	A	2000	EFZ	C13-C7	2.42	1.59	1.53
3	A	2000	EFZ	C2-C1	2.28	1.43	1.39
3	A	2000	EFZ	C12-C11	2.17	1.56	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	EFZ	O2-C14-N	6.40	122.27	116.88
3	A	2000	EFZ	O2-C7-C8	-4.96	101.04	107.86
3	A	2000	EFZ	O2-C7-C13	3.80	111.66	104.52
3	A	2000	EFZ	C7-O2-C14	-3.09	115.70	121.71
3	A	2000	EFZ	C6-C7-C8	-3.06	108.48	112.23
3	A	2000	EFZ	O2-C7-C6	2.85	113.80	111.60
3	A	2000	EFZ	C12-C10-C9	-2.63	109.69	119.26
3	A	2000	EFZ	C1-N-C14	-2.27	121.76	123.97
3	A	2000	EFZ	C4-C5-C6	2.22	122.39	118.88
3	A	2000	EFZ	F2-C13-C7	-2.22	109.00	111.73
3	A	2000	EFZ	C5-C6-C7	2.20	125.51	122.69
3	A	2000	EFZ	O1-C14-N	-2.12	119.03	124.28

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2000	EFZ	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	A	2000	EFZ	C11-C10-C9-C8

There are no ring outliers.

## 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	557/560 (99%)	-0.32	1 (0%) 93 54	33, 73, 115, 148	2 (0%)
2	B	405/427 (94%)	-0.35	0 100 100	37, 65, 134, 147	9 (2%)
All	All	962/987 (97%)	-0.33	1 (0%) 93 63	33, 70, 126, 148	11 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	ALA	2.9

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	EFZ	A	2000	21/21	0.17	0.04	43,47,53,53	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.