



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:35 AM GMT

PDB ID : 1JKH  
Title : CRYSTAL STRUCTURE OF Y181C MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH DMP-266(EFAVIRENZ)  
Authors : Ren, J.; Nichols, C.; Bird, L.; Chamberlain, P.; Weaver, K.; Short, S.; Stuart, D.I.; Stammers, D.K.  
Deposited on : 2001-07-12  
Resolution : 2.50 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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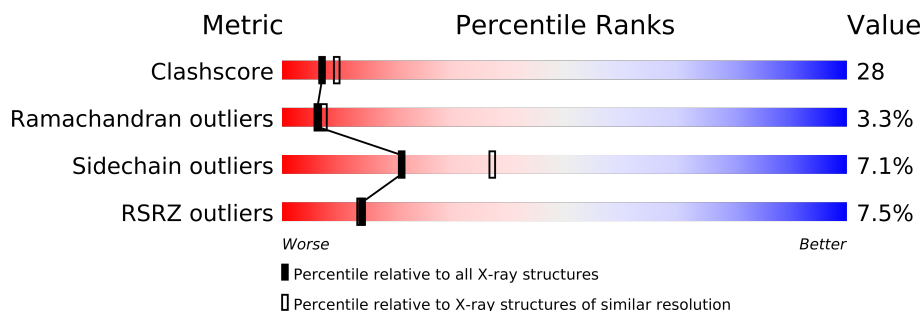
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 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	440	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7926 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 HIV-1 RT, A-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4491	2899	750	833	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	CYS	TYR	OXIDIZED CYS	UNP P04585
A	280	CSD	CYS	OXIDIZED CYS	UNP P04585

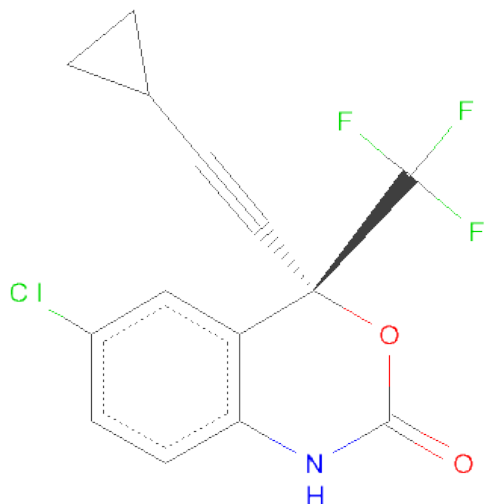
- Molecule 2 is a protein called HIV-1 RT, B-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	398	Total	C	N	O	S	0	0	0
			3291	2137	550	596	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	181	CYS	TYR	ENGINEERED	UNP P04585

- 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>).

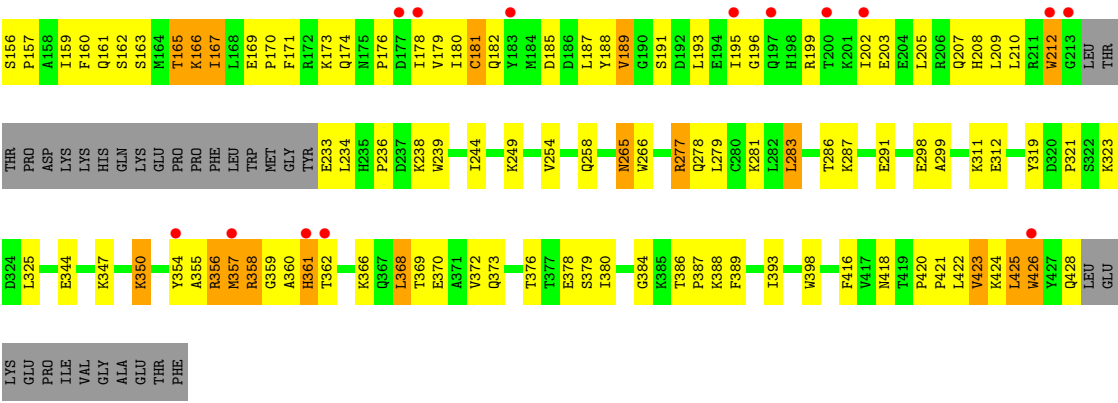


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
3	A	1	21	14	1	3	1	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	52	Total	O	0	0
			52	52		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.50Å 109.00Å 73.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 2.50 29.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.68-2.50) 98.7 (29.68-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.236 , 0.303 0.230 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.4	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	1 of 38614 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: 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	0.46	0/4596	0.70	1/6242 (0.0%)
2	B	0.42	0/3382	0.67	0/4591
All	All	0.45	0/7978	0.68	1/10833 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	GLY	N-CA-C	6.01	128.12	113.10

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	4491	0	4537	289	0
2	B	3291	0	3321	173	0
3	A	21	0	9	1	0
4	A	71	0	0	8	0
4	B	52	0	0	2	0
All	All	7926	0	7867	446	0



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 28.

All (446) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:50:ILE:HG13	1:A:51:GLY:H	1.12	1.11
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.23	1.02
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.44	0.99
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.48	0.95
2:B:350:LYS:HE2	2:B:378:GLU:OE2	1.67	0.94
1:A:50:ILE:HD12	1:A:52:PRO:HD2	1.51	0.91
1:A:50:ILE:CG1	1:A:51:GLY:H	1.85	0.89
1:A:23:GLN:O	1:A:25:PRO:HD3	1.73	0.89
1:A:19:PRO:HB3	1:A:56:TYR:CD1	2.12	0.85
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.12	0.84
1:A:65:LYS:HB3	1:A:68:SER:HB2	1.60	0.82
1:A:467:VAL:HG13	4:A:1037:HOH:O	1.77	0.82
2:B:98:ALA:HB1	2:B:101:LYS:HE3	1.60	0.82
1:A:111:VAL:HG22	1:A:185:ASP:O	1.80	0.81
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.16	0.81
1:A:126:LYS:H	1:A:126:LYS:HD2	1.46	0.80
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.46	0.79
1:A:334:GLN:O	1:A:356:ARG:HD3	1.83	0.79
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.17	0.78
1:A:206:ARG:HH11	1:A:216:THR:HG23	1.49	0.78
1:A:522:ILE:O	1:A:526:ILE:HG13	1.82	0.77
2:B:254:VAL:O	2:B:258:GLN:HG3	1.83	0.77
2:B:169:GLU:O	2:B:173:LYS:HD3	1.86	0.76
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.01	0.75
1:A:50:ILE:HG13	1:A:51:GLY:N	1.95	0.75
1:A:122:GLU:HA	1:A:125:ARG:NE	2.03	0.74
2:B:169:GLU:HA	2:B:173:LYS:HZ3	1.53	0.74
2:B:182:GLN:HB2	2:B:187:LEU:HD12	1.69	0.73
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.70	0.72
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.86	0.72
1:A:441:TYR:O	1:A:548:VAL:HG11	1.89	0.72
1:A:118:VAL:O	1:A:148:VAL:HB	1.88	0.72
2:B:169:GLU:HG2	2:B:173:LYS:NZ	2.05	0.71
2:B:376:THR:O	2:B:380:ILE:HG13	1.89	0.71
2:B:425:LEU:HA	2:B:428:GLN:HE21	1.56	0.71
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.72	0.71
1:A:96:HIS:HB2	4:A:1002:HOH:O	1.90	0.71
1:A:315:HIS:HB3	4:A:1058:HOH:O	1.91	0.70
1:A:52:PRO:O	1:A:53:GLU:HG3	1.91	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:399:GLU:O	1:A:403:THR:HB	1.92	0.70
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.27	0.70
2:B:100:LEU:HD22	2:B:181:CYS:HB2	1.74	0.69
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.75	0.69
2:B:6:GLU:O	2:B:7:THR:HG23	1.92	0.69
1:A:278:GLN:O	1:A:282:LEU:HD13	1.91	0.69
1:A:33:ALA:HB1	1:A:71:TRP:HB2	1.73	0.69
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.75	0.69
2:B:425:LEU:H	2:B:425:LEU:HD13	1.58	0.68
1:A:77:PHE:HD2	1:A:80:LEU:HD23	1.58	0.68
2:B:79:GLU:O	2:B:83:ARG:HG3	1.93	0.68
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.75	0.68
1:A:50:ILE:CD1	1:A:52:PRO:HD2	2.24	0.68
1:A:466:VAL:O	1:A:467:VAL:HG23	1.94	0.68
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.74	0.67
2:B:98:ALA:O	2:B:101:LYS:HG2	1.94	0.67
2:B:426:TRP:HZ3	4:B:1078:HOH:O	1.77	0.67
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.76	0.67
1:A:122:GLU:N	1:A:122:GLU:OE1	2.27	0.67
1:A:131:THR:HG22	1:A:132:ILE:N	2.09	0.67
1:A:324:ASP:O	1:A:343:GLN:HG2	1.94	0.67
2:B:84:THR:HB	2:B:154:LYS:HE2	1.76	0.66
1:A:293:ILE:HD12	1:A:293:ILE:N	2.11	0.66
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.31	0.65
2:B:113:ASP:O	2:B:116:PHE:HD2	1.78	0.65
1:A:37:ILE:O	1:A:40:GLU:HB3	1.97	0.65
2:B:203:GLU:O	2:B:207:GLN:HG2	1.94	0.65
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.77	0.65
1:A:135:ILE:H	1:A:135:ILE:HD12	1.60	0.65
2:B:33:ALA:O	2:B:37:ILE:HG13	1.96	0.65
1:A:129:ALA:HA	1:A:144:TYR:O	1.96	0.65
1:A:18:GLY:HA2	1:A:83:ARG:HD2	1.79	0.65
1:A:126:LYS:HD2	1:A:126:LYS:N	2.12	0.65
1:A:18:GLY:HA2	1:A:83:ARG:CD	2.27	0.65
2:B:249:LYS:HB2	2:B:249:LYS:HZ3	1.61	0.65
1:A:395:LYS:O	1:A:399:GLU:HB2	1.97	0.65
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.11	0.64
1:A:19:PRO:HA	1:A:56:TYR:HA	1.79	0.64
1:A:66:LYS:O	1:A:67:ASP:HB3	1.95	0.64
1:A:330:GLN:HB2	1:A:338:THR:OG1	1.98	0.64
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.28	0.64
1:A:57:ASN:HB2	1:A:143:ARG:NH2	2.06	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:161:GLN:O	2:B:165:THR:HG22	1.98	0.63
1:A:50:ILE:CG1	1:A:51:GLY:N	2.58	0.63
2:B:425:LEU:N	2:B:425:LEU:HD13	2.14	0.63
1:A:306:ASN:O	1:A:310:LEU:HG	1.98	0.63
1:A:468:THR:O	1:A:469:LEU:HD23	1.98	0.63
2:B:163:SER:O	2:B:167:ILE:HG23	1.98	0.63
2:B:5:ILE:HD13	2:B:5:ILE:N	2.13	0.63
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.80	0.63
2:B:278:GLN:HE21	2:B:298:GLU:HB3	1.64	0.62
2:B:10:VAL:HG21	2:B:159:ILE:HD11	1.80	0.62
1:A:72:ARG:HD3	1:A:73:LYS:H	1.64	0.62
2:B:422:LEU:O	2:B:424:LYS:N	2.32	0.62
1:A:120:LEU:HD23	1:A:121:ASP:H	1.64	0.62
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.34	0.61
1:A:122:GLU:HG2	1:A:123:ASP:H	1.64	0.61
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.30	0.61
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.83	0.61
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.82	0.61
1:A:518:VAL:O	1:A:522:ILE:HG13	2.01	0.60
1:A:438:GLU:HB2	1:A:461:ARG:NH1	2.15	0.60
1:A:94:ILE:H	1:A:94:ILE:HD13	1.66	0.60
1:A:18:GLY:CA	1:A:83:ARG:HD2	2.31	0.60
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.82	0.60
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.83	0.60
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.82	0.60
1:A:31:ILE:O	1:A:35:VAL:HG23	2.01	0.60
1:A:210:LEU:HD21	1:A:215:THR:HA	1.83	0.60
2:B:368:LEU:O	2:B:372:VAL:HG23	2.02	0.60
2:B:323:LYS:HB2	2:B:323:LYS:NZ	2.17	0.60
1:A:52:PRO:C	1:A:53:GLU:HG3	2.23	0.59
2:B:169:GLU:HG2	2:B:173:LYS:HZ1	1.67	0.59
1:A:548:VAL:O	1:A:552:VAL:HG22	2.01	0.59
2:B:311:LYS:O	2:B:312:GLU:HG3	2.02	0.59
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.38	0.58
2:B:356:ARG:CD	2:B:357:MET:H	2.16	0.58
1:A:131:THR:CG2	1:A:132:ILE:N	2.66	0.58
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.85	0.58
1:A:48:SER:HB2	1:A:147:ASN:HD21	1.68	0.58
2:B:422:LEU:HG	2:B:426:TRP:CZ2	2.38	0.58
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.03	0.58
1:A:454:LYS:NZ	1:A:554:ALA:HB3	2.19	0.58
1:A:58:THR:O	1:A:130:PHE:HB2	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:392:PRO:O	1:A:423:VAL:HG13	2.04	0.58
1:A:435:VAL:HG23	4:A:1035:HOH:O	2.02	0.58
1:A:122:GLU:HG2	1:A:123:ASP:N	2.19	0.58
2:B:380:ILE:O	2:B:384:GLY:N	2.35	0.58
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.52	0.58
1:A:58:THR:HG23	1:A:76:ASP:O	2.03	0.57
1:A:58:THR:HG21	1:A:75:VAL:HG12	1.87	0.57
2:B:376:THR:CG2	2:B:386:THR:HG22	2.34	0.57
2:B:422:LEU:HA	2:B:425:LEU:HD22	1.85	0.57
1:A:59:PRO:HG2	1:A:76:ASP:HB2	1.86	0.57
1:A:37:ILE:HD11	1:A:71:TRP:O	2.04	0.57
1:A:376:THR:HG23	1:A:386:THR:HG23	1.85	0.57
2:B:118:VAL:HB	2:B:149:LEU:HG	1.84	0.57
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.86	0.57
1:A:178:ILE:HD12	1:A:178:ILE:N	2.20	0.57
1:A:109:LEU:HG	1:A:216:THR:OG1	2.04	0.56
2:B:376:THR:HG23	2:B:386:THR:HG22	1.86	0.56
2:B:10:VAL:CG2	2:B:159:ILE:HD11	2.35	0.56
2:B:354:TYR:OH	2:B:357:MET:HG3	2.05	0.56
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.88	0.56
1:A:194:GLU:HG2	1:A:197:GLN:OE1	2.05	0.56
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.40	0.56
1:A:106:VAL:HG23	1:A:236:PRO:HB3	1.86	0.56
1:A:39:THR:O	1:A:43:LYS:HG3	2.05	0.56
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.40	0.56
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.41	0.56
1:A:126:LYS:H	1:A:126:LYS:CD	2.18	0.56
1:A:50:ILE:HB	1:A:145:GLN:HG2	1.86	0.56
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.41	0.56
1:A:147:ASN:ND2	4:A:1098:HOH:O	2.38	0.56
2:B:163:SER:HA	2:B:166:LYS:HD3	1.86	0.56
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.36	0.56
1:A:260:LEU:O	1:A:264:LEU:HD23	2.05	0.56
1:A:124:PHE:O	1:A:127:TYR:HD2	1.89	0.56
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.87	0.56
1:A:9:PRO:HG2	2:B:53:GLU:HG3	1.89	0.55
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.89	0.55
1:A:12:LEU:HD13	1:A:17:ASP:HA	1.88	0.55
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.89	0.55
1:A:458:VAL:HG23	1:A:548:VAL:HG12	1.87	0.55
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.88	0.55
1:A:443:ASP:OD1	1:A:444:GLY:N	2.40	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.71	0.55
1:A:94:ILE:HG13	1:A:230:MET:CE	2.37	0.55
2:B:113:ASP:O	2:B:116:PHE:CD2	2.60	0.55
1:A:219:LYS:HD3	1:A:219:LYS:O	2.06	0.55
1:A:51:GLY:N	1:A:52:PRO:CD	2.70	0.54
1:A:7:THR:HG21	1:A:120:LEU:O	2.08	0.54
1:A:402:TRP:CD1	1:A:402:TRP:C	2.80	0.54
1:A:84:THR:O	1:A:154:LYS:NZ	2.38	0.54
2:B:298:GLU:N	2:B:298:GLU:OE1	2.39	0.54
1:A:479:LEU:HD11	1:A:501:TYR:HE2	1.73	0.54
1:A:253:THR:O	1:A:257:ILE:HG13	2.07	0.54
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.89	0.54
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.89	0.54
2:B:236:PRO:C	2:B:238:LYS:H	2.11	0.54
1:A:132:ILE:HB	1:A:142:ILE:HB	1.90	0.54
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.90	0.54
1:A:538:ALA:O	1:A:545:ASN:ND2	2.41	0.53
1:A:142:ILE:HG22	1:A:144:TYR:CE1	2.44	0.53
2:B:122:GLU:HA	2:B:125:ARG:CD	2.39	0.53
1:A:114:ALA:CB	1:A:160:PHE:CE2	2.89	0.53
1:A:111:VAL:HG11	1:A:164:MET:HE1	1.90	0.53
2:B:369:THR:O	2:B:373:GLN:HG3	2.08	0.53
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.91	0.53
2:B:22:LYS:HE3	4:B:1068:HOH:O	2.07	0.53
1:A:112:GLY:O	1:A:114:ALA:N	2.38	0.53
1:A:121:ASP:O	1:A:122:GLU:C	2.47	0.53
1:A:238:LYS:HB2	1:A:316:GLY:O	2.08	0.53
1:A:458:VAL:HG23	1:A:548:VAL:CG1	2.40	0.52
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.42	0.52
1:A:460:ASN:O	1:A:461:ARG:CB	2.57	0.52
2:B:78:ARG:O	2:B:82:LYS:HG3	2.09	0.52
1:A:120:LEU:CD2	1:A:121:ASP:H	2.22	0.52
2:B:359:GLY:HA2	2:B:361:HIS:CE1	2.45	0.52
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.39	0.52
1:A:31:ILE:HD13	1:A:134:SER:HA	1.92	0.52
1:A:540:LYS:HB3	1:A:542:ILE:HG13	1.92	0.52
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.44	0.52
1:A:363:ASN:HA	1:A:511:ASP:CG	2.30	0.52
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.09	0.52
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.45	0.52
1:A:340:GLN:CB	1:A:351:THR:HG22	2.39	0.52
2:B:178:ILE:HG21	2:B:189:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:51:GLY:N	1:A:52:PRO:HD2	2.24	0.52
1:A:206:ARG:O	1:A:210:LEU:HD23	2.10	0.52
1:A:540:LYS:C	1:A:542:ILE:H	2.13	0.51
2:B:191:SER:CB	2:B:193:LEU:HD13	2.39	0.51
1:A:210:LEU:HD22	1:A:214:LEU:O	2.10	0.51
2:B:179:VAL:O	2:B:189:VAL:HA	2.11	0.51
1:A:37:ILE:HD13	1:A:72:ARG:NH1	2.26	0.51
2:B:24:TRP:HB2	2:B:25:PRO:HD2	1.93	0.51
1:A:19:PRO:HB3	1:A:56:TYR:CG	2.46	0.51
2:B:355:ALA:O	2:B:356:ARG:HG3	2.10	0.51
1:A:254:VAL:HG13	1:A:283:LEU:HD12	1.92	0.51
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.93	0.51
2:B:27:THR:O	2:B:31:ILE:HG13	2.11	0.51
1:A:226:PRO:HA	1:A:234:LEU:O	2.11	0.51
2:B:170:PRO:O	2:B:174:GLN:HG3	2.10	0.50
2:B:162:SER:O	2:B:165:THR:HG23	2.11	0.50
1:A:408:ALA:HB3	2:B:393:ILE:CG1	2.41	0.50
1:A:460:ASN:O	1:A:461:ARG:HB2	2.10	0.50
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.41	0.50
1:A:253:THR:HA	1:A:291:GLU:O	2.10	0.50
1:A:402:TRP:CH2	2:B:362:THR:HA	2.47	0.50
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.93	0.50
2:B:70:LYS:HB2	2:B:70:LYS:NZ	2.26	0.50
1:A:378:GLU:O	1:A:382:ILE:HG12	2.12	0.50
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.92	0.50
1:A:329:ILE:HG22	1:A:330:GLN:N	2.26	0.50
2:B:65:LYS:NZ	2:B:110:ASP:OD1	2.44	0.50
1:A:486:LEU:O	1:A:528:LYS:NZ	2.41	0.50
1:A:63:ILE:HD12	1:A:63:ILE:N	2.27	0.50
2:B:169:GLU:HG2	2:B:173:LYS:HZ3	1.77	0.50
1:A:385:LYS:HB3	1:A:385:LYS:NZ	2.27	0.50
2:B:239:TRP:CE3	2:B:378:GLU:HG3	2.46	0.50
1:A:210:LEU:CD2	1:A:215:THR:HA	2.41	0.50
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.59	0.50
1:A:452:LEU:HD23	1:A:470:THR:HA	1.94	0.49
1:A:235:HIS:HB2	1:A:238:LYS:O	2.13	0.49
1:A:329:ILE:O	1:A:392:PRO:HD3	2.12	0.49
1:A:500:GLN:OE1	2:B:422:LEU:HD22	2.13	0.49
2:B:425:LEU:N	2:B:425:LEU:CD1	2.75	0.49
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.95	0.49
1:A:475:GLN:HB3	1:A:501:TYR:CD2	2.47	0.49
2:B:202:ILE:O	2:B:205:LEU:N	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:60:VAL:HG12	2:B:75:VAL:HG13	1.95	0.49
1:A:292:VAL:C	1:A:293:ILE:HD12	2.32	0.49
1:A:100:LEU:O	1:A:318:TYR:HB3	2.12	0.49
2:B:40:GLU:O	2:B:44:GLU:HG3	2.13	0.49
1:A:31:ILE:CG1	1:A:133:PRO:HG2	2.42	0.48
2:B:57:ASN:ND2	2:B:143:ARG:HH11	2.10	0.48
1:A:136:ASN:O	1:A:137:ASN:C	2.50	0.48
1:A:123:ASP:O	1:A:126:LYS:HD3	2.12	0.48
1:A:41:MET:CE	1:A:73:LYS:HE3	2.43	0.48
1:A:474:ASN:O	1:A:478:GLU:HG2	2.14	0.48
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.49	0.48
2:B:87:PHE:CE2	2:B:155:GLY:HA2	2.48	0.48
1:A:229:TRP:CD1	1:A:230:MET:HG2	2.49	0.48
1:A:138:GLU:HG2	1:A:138:GLU:O	2.14	0.48
1:A:20:LYS:HB3	1:A:21:VAL:H	1.51	0.48
1:A:19:PRO:O	1:A:20:LYS:HG3	2.14	0.48
1:A:111:VAL:HG21	1:A:160:PHE:HZ	1.78	0.48
1:A:466:VAL:O	1:A:467:VAL:CG2	2.61	0.48
1:A:94:ILE:HG13	1:A:230:MET:HE2	1.95	0.48
2:B:82:LYS:NZ	2:B:82:LYS:CB	2.77	0.48
2:B:209:LEU:O	2:B:212:TRP:HB2	2.14	0.48
1:A:121:ASP:O	1:A:123:ASP:N	2.47	0.48
1:A:12:LEU:O	1:A:13:LYS:C	2.53	0.48
1:A:537:PRO:HB3	2:B:265:ASN:ND2	2.29	0.48
1:A:111:VAL:HG11	1:A:164:MET:CE	2.44	0.47
1:A:260:LEU:O	1:A:264:LEU:CD2	2.61	0.47
1:A:479:LEU:HD11	1:A:501:TYR:CE2	2.50	0.47
1:A:421:PRO:HG3	4:A:1025:HOH:O	2.15	0.47
1:A:547:GLN:HG3	2:B:286:THR:HG22	1.97	0.47
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.44	0.47
1:A:454:LYS:HZ1	1:A:554:ALA:HB3	1.79	0.47
1:A:486:LEU:HB3	1:A:524:GLN:HB3	1.96	0.47
2:B:44:GLU:OE1	2:B:46:LYS:HE3	2.14	0.47
1:A:19:PRO:CA	1:A:56:TYR:HA	2.45	0.47
2:B:278:GLN:HE21	2:B:298:GLU:CB	2.25	0.47
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.48	0.47
1:A:206:ARG:HB3	1:A:206:ARG:NH1	2.30	0.47
2:B:195:ILE:HG23	2:B:196:GLY:N	2.30	0.47
1:A:194:GLU:HG3	1:A:197:GLN:HB2	1.97	0.47
1:A:149:LEU:HG	1:A:156:SER:HA	1.97	0.47
2:B:278:GLN:OE1	2:B:278:GLN:HA	2.15	0.47
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:277:ARG:O	2:B:281:LYS:HG3	2.15	0.47
1:A:115:TYR:O	1:A:149:LEU:HB2	2.14	0.46
1:A:307:ARG:O	1:A:311:LYS:HG3	2.15	0.46
1:A:170:PRO:HA	1:A:173:LYS:HD3	1.97	0.46
1:A:466:VAL:HG21	1:A:551:LEU:HB3	1.96	0.46
1:A:368:LEU:HD12	1:A:423:VAL:HG21	1.96	0.46
1:A:30:LYS:CD	1:A:62:ALA:HB3	2.41	0.46
2:B:61:PHE:CD2	2:B:61:PHE:N	2.83	0.46
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.98	0.46
2:B:180:ILE:HA	2:B:188:TYR:O	2.16	0.46
1:A:279:LEU:O	1:A:282:LEU:HB2	2.16	0.46
1:A:547:GLN:O	1:A:550:LYS:HB2	2.15	0.46
2:B:350:LYS:HB3	2:B:350:LYS:HE3	1.73	0.46
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.51	0.46
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.51	0.45
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.99	0.45
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.51	0.45
1:A:468:THR:C	1:A:469:LEU:HD23	2.37	0.45
1:A:319:TYR:OH	1:A:385:LYS:HD3	2.16	0.45
1:A:357:MET:N	4:A:1063:HOH:O	2.49	0.45
1:A:11:LYS:O	1:A:85:GLN:HB3	2.16	0.45
1:A:94:ILE:HD13	1:A:94:ILE:N	2.30	0.45
2:B:162:SER:O	2:B:165:THR:CG2	2.65	0.45
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.52	0.45
2:B:171:PHE:CG	2:B:205:LEU:HD23	2.52	0.45
1:A:543:GLY:HA3	2:B:283:LEU:O	2.16	0.45
1:A:438:GLU:CD	1:A:461:ARG:HD2	2.37	0.45
2:B:356:ARG:HH11	2:B:356:ARG:CG	2.30	0.45
2:B:210:LEU:C	2:B:212:TRP:H	2.21	0.45
2:B:344:GLU:HB2	2:B:347:LYS:HE3	1.99	0.45
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.98	0.45
1:A:519:ASN:O	1:A:523:GLU:HG2	2.17	0.45
1:A:546:GLU:O	1:A:550:LYS:HG3	2.17	0.45
2:B:97:PRO:C	2:B:99:GLY:N	2.70	0.44
1:A:332:GLN:HG2	1:A:332:GLN:O	2.17	0.44
2:B:234:LEU:N	2:B:234:LEU:HD12	2.32	0.44
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.99	0.44
1:A:50:ILE:HG23	1:A:51:GLY:N	2.32	0.44
1:A:94:ILE:HG21	1:A:183:TYR:HE2	1.81	0.44
1:A:94:ILE:HG13	1:A:230:MET:HE1	1.99	0.44
2:B:56:TYR:HE2	2:B:126:LYS:CE	2.29	0.44
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.81	0.44
1:A:229:TRP:HB2	1:A:234:LEU:HD22	2.00	0.44
1:A:259:LYS:HD3	1:A:259:LYS:N	2.32	0.44
1:A:19:PRO:O	1:A:20:LYS:CG	2.66	0.44
2:B:97:PRO:C	2:B:99:GLY:H	2.21	0.44
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.53	0.44
1:A:119:PRO:HA	1:A:148:VAL:HG12	1.99	0.44
2:B:29:GLU:HG2	2:B:71:TRP:CZ2	2.53	0.44
1:A:346:PHE:N	1:A:346:PHE:CD2	2.83	0.44
2:B:70:LYS:HG3	2:B:70:LYS:H	1.50	0.44
1:A:21:VAL:HG13	1:A:21:VAL:O	2.18	0.44
1:A:407:GLN:CG	2:B:393:ILE:HA	2.47	0.44
1:A:19:PRO:O	1:A:20:LYS:CB	2.66	0.43
1:A:126:LYS:HB3	1:A:126:LYS:HE3	1.82	0.43
1:A:460:ASN:O	1:A:460:ASN:OD1	2.36	0.43
1:A:38:CYS:O	1:A:47:ILE:HD11	2.18	0.43
2:B:153:TRP:O	2:B:157:PRO:HD2	2.18	0.43
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.99	0.43
1:A:249:LYS:HE3	1:A:249:LYS:HB2	1.84	0.43
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.66	0.43
2:B:169:GLU:C	2:B:173:LYS:HD3	2.37	0.43
1:A:378:GLU:O	1:A:381:VAL:HB	2.18	0.43
1:A:464:GLN:O	1:A:465:LYS:HB2	2.18	0.43
2:B:422:LEU:HD23	2:B:426:TRP:HE1	1.83	0.43
2:B:39:THR:O	2:B:43:LYS:HG2	2.18	0.43
1:A:8:VAL:HG21	1:A:159:ILE:HG23	2.00	0.43
1:A:202:ILE:O	1:A:206:ARG:HG3	2.18	0.43
1:A:17:ASP:O	1:A:83:ARG:HD3	2.18	0.43
1:A:58:THR:CG2	1:A:75:VAL:HG12	2.48	0.43
2:B:207:GLN:HA	2:B:207:GLN:OE1	2.19	0.43
2:B:236:PRO:C	2:B:238:LYS:N	2.71	0.43
2:B:156:SER:N	2:B:157:PRO:HD2	2.34	0.43
1:A:184:MET:HB3	1:A:185:ASP:H	1.60	0.43
2:B:101:LYS:HG3	2:B:102:LYS:HG3	2.01	0.43
1:A:72:ARG:HD3	1:A:73:LYS:N	2.32	0.43
1:A:111:VAL:HG22	1:A:185:ASP:C	2.37	0.43
2:B:266:TRP:CH2	2:B:426:TRP:HB3	2.53	0.43
1:A:293:ILE:CD1	1:A:293:ILE:N	2.80	0.43
1:A:405:TYR:HE2	1:A:407:GLN:HB3	1.83	0.43
2:B:205:LEU:HD13	2:B:209:LEU:HD22	2.00	0.43
1:A:457:TYR:CE1	1:A:464:GLN:HA	2.54	0.43
1:A:410:TRP:CG	1:A:411:ILE:N	2.87	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:387:PRO:HG2	2:B:389:PHE:HE1	1.76	0.42
1:A:12:LEU:HD11	1:A:127:TYR:CD1	2.54	0.42
1:A:498:ASP:HB2	1:A:538:ALA:HA	2.01	0.42
1:A:393:ILE:HG12	1:A:394:GLN:N	2.34	0.42
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.77	0.42
1:A:122:GLU:HA	1:A:125:ARG:CD	2.48	0.42
1:A:329:ILE:CG2	1:A:330:GLN:N	2.83	0.42
1:A:500:GLN:HE21	1:A:500:GLN:HB3	1.72	0.42
1:A:24:TRP:O	1:A:25:PRO:C	2.58	0.42
1:A:466:VAL:HG12	1:A:467:VAL:N	2.33	0.42
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.34	0.42
2:B:234:LEU:N	2:B:234:LEU:CD1	2.83	0.42
1:A:102:LYS:O	1:A:103:LYS:HD3	2.19	0.42
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.55	0.42
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.54	0.42
1:A:271:TYR:CE1	1:A:314:VAL:CG2	3.02	0.42
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.55	0.42
1:A:122:GLU:HA	1:A:125:ARG:HE	1.81	0.42
1:A:8:VAL:HG13	2:B:53:GLU:OE1	2.20	0.42
1:A:69:THR:HG22	1:A:69:THR:O	2.20	0.42
1:A:305:GLU:O	1:A:309:ILE:HG13	2.20	0.42
2:B:173:LYS:N	2:B:173:LYS:HD2	2.34	0.41
2:B:173:LYS:O	2:B:176:PRO:HD3	2.19	0.41
1:A:282:LEU:HD11	1:A:296:THR:HG23	2.02	0.41
2:B:116:PHE:CD1	2:B:116:PHE:C	2.94	0.41
2:B:279:LEU:HD23	2:B:299:ALA:HB1	2.01	0.41
1:A:113:ASP:OD1	1:A:113:ASP:O	2.37	0.41
2:B:6:GLU:O	2:B:7:THR:CG2	2.64	0.41
2:B:356:ARG:HH11	2:B:356:ARG:HG3	1.85	0.41
2:B:360:ALA:CB	2:B:366:LYS:HD3	2.50	0.41
1:A:357:MET:HE3	1:A:367:GLN:HE22	1.85	0.41
1:A:179:VAL:HG13	4:A:1007:HOH:O	2.19	0.41
1:A:57:ASN:HA	1:A:129:ALA:O	2.20	0.41
1:A:178:ILE:N	1:A:178:ILE:CD1	2.83	0.41
1:A:323:LYS:HB2	1:A:343:GLN:NE2	2.36	0.41
2:B:323:LYS:HZ3	2:B:323:LYS:HB2	1.85	0.41
1:A:492:GLU:HA	1:A:530:LYS:O	2.21	0.41
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.51	0.41
2:B:88:TRP:CE3	2:B:88:TRP:HA	2.55	0.41
1:A:32:LYS:HD3	1:A:32:LYS:HA	1.87	0.41
2:B:366:LYS:O	2:B:370:GLU:HG3	2.21	0.41
1:A:545:ASN:O	1:A:549:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:169:GLU:O	1:A:173:LYS:HD3	2.21	0.41
1:A:205:LEU:HD22	1:A:209:LEU:HD11	2.02	0.41
2:B:393:ILE:O	2:B:416:PHE:HB3	2.21	0.41
1:A:236:PRO:HA	3:A:999:EFZ:H3	2.02	0.41
1:A:486:LEU:HD12	1:A:521:ILE:HG23	2.01	0.41
2:B:88:TRP:CE3	2:B:88:TRP:CA	3.03	0.41
1:A:536:VAL:HG12	2:B:258:GLN:HB3	2.02	0.41
1:A:94:ILE:CG2	1:A:183:TYR:HE2	2.33	0.41
2:B:360:ALA:O	2:B:362:THR:N	2.54	0.41
1:A:539:HIS:O	1:A:540:LYS:HD2	2.21	0.41
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	0.41
1:A:438:GLU:CG	1:A:439:THR:N	2.84	0.41
1:A:30:LYS:HE2	1:A:71:TRP:CZ3	2.55	0.40
1:A:41:MET:HE3	1:A:73:LYS:HE3	2.03	0.40
1:A:546:GLU:CG	1:A:547:GLN:NE2	2.84	0.40
1:A:131:THR:HG23	1:A:142:ILE:O	2.21	0.40
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.79	0.40
1:A:120:LEU:HB2	1:A:148:VAL:HA	2.03	0.40
2:B:49:LYS:HA	2:B:143:ARG:O	2.22	0.40
2:B:97:PRO:HD2	2:B:181:CYS:SG	2.62	0.40
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.50	0.40
2:B:87:PHE:O	2:B:88:TRP:C	2.59	0.40
2:B:64:LYS:HE2	2:B:69:THR:O	2.21	0.40
1:A:115:TYR:CD1	1:A:151:GLN:NE2	2.89	0.40
2:B:195:ILE:HG12	2:B:199:ARG:NH2	2.37	0.40
1:A:412:PRO:O	1:A:413:GLU:C	2.60	0.40
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.98	0.40
2:B:125:ARG:HB3	2:B:145:GLN:NE2	2.36	0.40
1:A:102:LYS:HG3	1:A:237:ASP:HA	2.04	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	546/560 (98%)	475 (87%)	47 (9%)	24 (4%)	4	4
2	B	392/440 (89%)	348 (89%)	37 (9%)	7 (2%)	13	20
All	All	938/1000 (94%)	823 (88%)	84 (9%)	31 (3%)	6	7

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	21	VAL
1	A	113	ASP
1	A	461	ARG
1	A	538	ALA
2	B	358	ARG
2	B	423	VAL
1	A	4	PRO
1	A	112	GLY
1	A	122	GLU
2	B	66	LYS
2	B	361	HIS
1	A	16	MET
1	A	129	ALA
1	A	137	ASN
1	A	183	TYR
1	A	465	LYS
1	A	19	PRO
1	A	52	PRO
1	A	78	ARG
1	A	528	LYS
1	A	91	GLN
1	A	361	HIS
2	B	166	LYS
2	B	212	TRP
2	B	357	MET
1	A	24	TRP
1	A	195	ILE
1	A	345	PRO
1	A	543	GLY
1	A	552	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/499 (99%)	455 (92%)	37 (8%)	19	34
2	B	362/400 (90%)	338 (93%)	24 (7%)	24	41
All	All	854/899 (95%)	793 (93%)	61 (7%)	21	37

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	52	PRO
1	A	66	LYS
1	A	67	ASP
1	A	86	ASP
1	A	89	GLU
1	A	91	GLN
1	A	92	LEU
1	A	94	ILE
1	A	120	LEU
1	A	126	LYS
1	A	136	ASN
1	A	138	GLU
1	A	143	ARG
1	A	145	GLN
1	A	151	GLN
1	A	184	MET
1	A	194	GLU
1	A	205	LEU
1	A	216	THR
1	A	218	ASP
1	A	222	GLN
1	A	234	LEU
1	A	238	LYS
1	A	249	LYS
1	A	324	ASP
1	A	340	GLN
1	A	362	THR
1	A	368	LEU

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Mol	Chain	Res	Type
1	A	402	TRP
1	A	403	THR
1	A	423	VAL
1	A	459	THR
1	A	474	ASN
1	A	496	VAL
1	A	517	LEU
1	A	529	GLU
2	B	5	ILE
2	B	40	GLU
2	B	61	PHE
2	B	70	LYS
2	B	88	TRP
2	B	113	ASP
2	B	165	THR
2	B	167	ILE
2	B	181	CYS
2	B	189	VAL
2	B	233	GLU
2	B	265	ASN
2	B	277	ARG
2	B	283	LEU
2	B	287	LYS
2	B	291	GLU
2	B	325	LEU
2	B	350	LYS
2	B	356	ARG
2	B	358	ARG
2	B	368	LEU
2	B	388	LYS
2	B	425	LEU
2	B	426	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	136	ASN
1	A	145	GLN
1	A	147	ASN
1	A	151	GLN
1	A	174	GLN

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Mol	Chain	Res	Type
1	A	208	HIS
1	A	221	HIS
1	A	255	ASN
1	A	278	GLN
1	A	334	GLN
1	A	336	GLN
1	A	361	HIS
1	A	367	GLN
1	A	474	ASN
1	A	547	GLN
2	B	57	ASN
2	B	175	ASN
2	B	197	GLN
2	B	208	HIS
2	B	265	ASN
2	B	332	GLN
2	B	336	GLN
2	B	394	GLN
2	B	428	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	7,7,8	6.84	2 (28%)	6,8,10	5.32	4 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	280	1	-	1/3/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	O-C	17.64	1.23	1.11
1	A	280	CSD	CA-C	2.97	1.53	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	CA-CB-SG	10.20	125.38	110.82
1	A	280	CSD	OD2-SG-OD1	5.23	118.08	109.39
1	A	280	CSD	OD1-SG-CB	4.52	117.23	105.25
1	A	280	CSD	C-CA-N	-3.79	110.04	113.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

## 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	999	-	23,23,23	2.41	9 (39%)	36,36,36	1.18	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	-	-	1/14/32/32	0/0/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	EFZ	C10-C9	5.74	1.70	1.46
3	A	999	EFZ	C12-C11	-5.52	1.28	1.48
3	A	999	EFZ	C7-C6	4.51	1.57	1.51
3	A	999	EFZ	C11-C10	-2.96	1.24	1.46
3	A	999	EFZ	C12-C10	-2.96	1.24	1.46
3	A	999	EFZ	C1-N	2.71	1.44	1.39
3	A	999	EFZ	C13-C7	2.14	1.58	1.53
3	A	999	EFZ	O2-C14	2.12	1.38	1.36
3	A	999	EFZ	C14-N	2.06	1.39	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	EFZ	C12-C10-C9	-3.75	105.59	119.26
3	A	999	EFZ	C11-C10-C9	-3.74	105.65	119.26

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	EFZ	C12-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	551/560 (98%)	0.31	45 (8%)	12 11	32, 67, 127, 150	0
2	B	398/440 (90%)	0.20	26 (6%)	18 18	34, 64, 119, 143	0
All	All	949/1000 (94%)	0.26	71 (7%)	14 14	32, 66, 124, 150	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	LYS	6.8
2	B	5	ILE	6.8
1	A	67	ASP	6.2
1	A	19	PRO	6.1
1	A	71	TRP	5.4
2	B	357	MET	4.9
1	A	74	LEU	4.8
2	B	178	ILE	4.5
1	A	22	LYS	4.5
1	A	66	LYS	4.5
2	B	67	ASP	4.3
1	A	28	GLU	4.3
1	A	92	LEU	4.3
1	A	448	ARG	4.3
2	B	88	TRP	4.2
1	A	69	THR	4.1
1	A	29	GLU	4.1
1	A	54	ASN	3.9
2	B	195	ILE	3.8
2	B	213	GLY	3.7
1	A	65	LYS	3.7
1	A	68	SER	3.6
1	A	52	PRO	3.6
1	A	24	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	61	PHE	3.3
2	B	66	LYS	3.3
1	A	132	ILE	3.2
1	A	245	VAL	3.1
1	A	554	ALA	3.1
1	A	63	ILE	3.1
2	B	212	TRP	3.0
2	B	69	THR	3.0
2	B	96	HIS	3.0
2	B	87	PHE	3.0
1	A	550	LYS	2.9
1	A	3	SER	2.9
1	A	136	ASN	2.8
1	A	138	GLU	2.8
1	A	56	TYR	2.8
1	A	26	LEU	2.8
1	A	21	VAL	2.7
1	A	73	LYS	2.7
2	B	361	HIS	2.6
1	A	72	ARG	2.6
2	B	43	LYS	2.6
2	B	354	TYR	2.6
1	A	139	THR	2.4
1	A	43	LYS	2.4
1	A	137	ASN	2.3
2	B	177	ASP	2.3
2	B	183	TYR	2.3
1	A	452	LEU	2.3
1	A	130	PHE	2.3
2	B	362	THR	2.3
1	A	469	LEU	2.3
1	A	64	LYS	2.3
1	A	135	ILE	2.2
2	B	200	THR	2.2
1	A	451	LYS	2.2
2	B	70	LYS	2.2
2	B	102	LYS	2.2
1	A	484	LEU	2.2
1	A	51	GLY	2.2
2	B	104	LYS	2.2
2	B	197	GLN	2.2
2	B	202	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	53	GLU	2.1
1	A	116	PHE	2.1
2	B	65	LYS	2.1
1	A	33	ALA	2.0
2	B	426	TRP	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. 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
1	CSD	A	280	8/9	0.13	-0.37	59,61,78,82	0

## 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	999	21/21	0.14	-0.10	31,55,65,70	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.