



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 12:58 am GMT

PDB ID : 1JKH  
Title : CRYSTAL STRUCTURE OF Y181C MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH DMP-266(EFAVIRENZ)  
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Deposited on : 2001-07-12  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

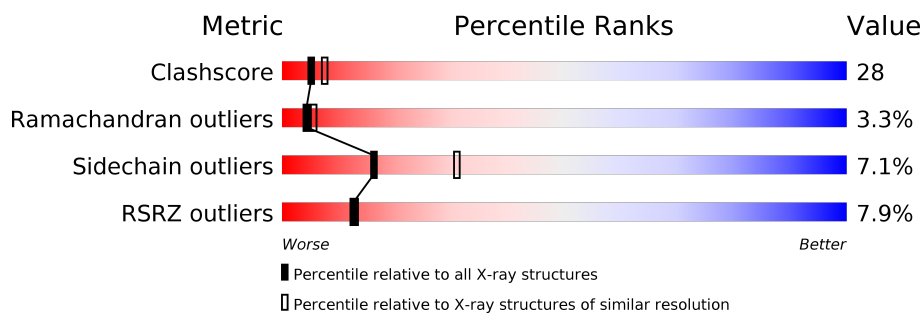
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (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. 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	
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 hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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

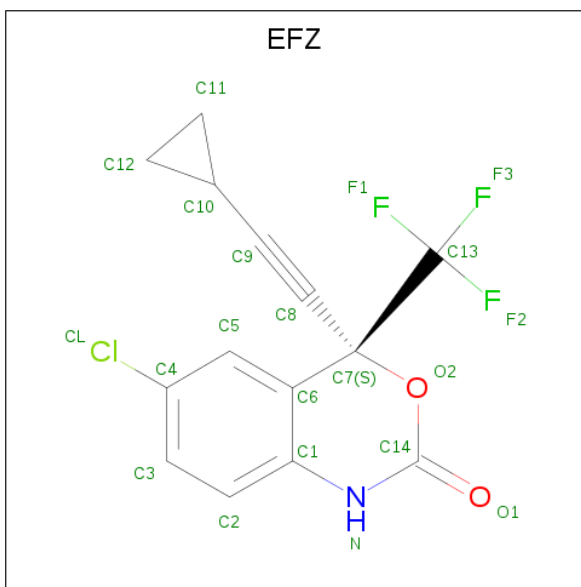
- Molecule 2 is a protein called HIV-1 RT, B-CHAIN.

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
3	A	1	Total	C	Cl	F	N	O	0	0
			21	14	1	3	1	2		

- Molecule 4 is water.

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

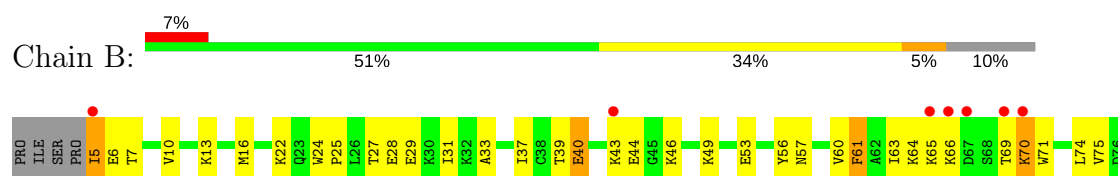
### 3 Residue-property plots

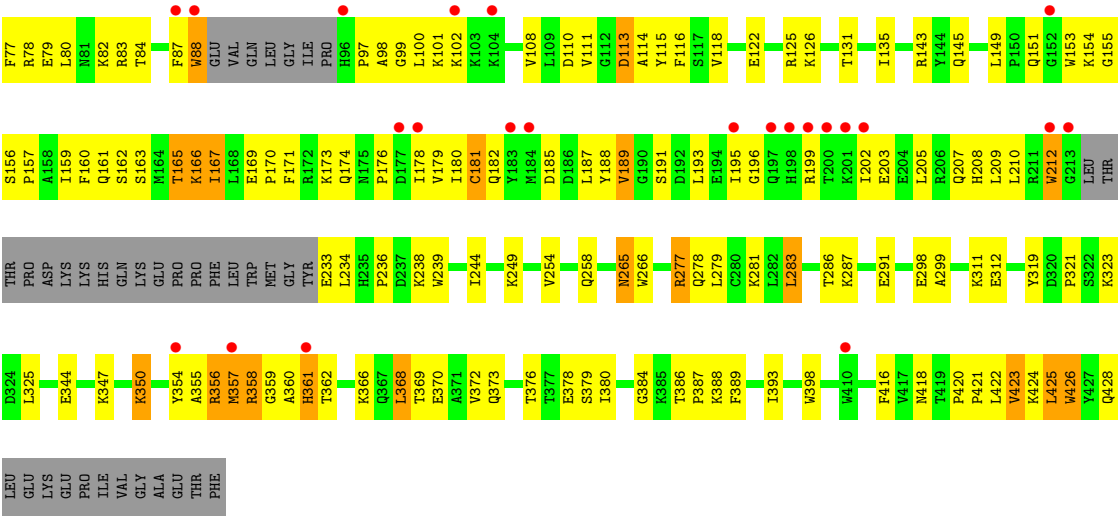
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: HIV-1 RT, A-CHAIN



#### • Molecule 2: HIV-1 RT, B-CHAIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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	Depositor
R, $R_{free}$	0.236 , 0.303 0.224 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
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> )	0.31 , 65.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	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.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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	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

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 28.

All (446) 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: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:467:VAL:HG13	4:A:1037:HOH:O	1.77	0.82
1:A:65:LYS:HB3	1:A:68:SER:HB2	1.60	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
1:A:441:TYR:O	1:A:548:VAL:HG11	1.89	0.72
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PRO:O	1:A:53:GLU:HG3	1.91	0.70
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.27	0.70
1:A:399:GLU:O	1:A:403:THR:HB	1.92	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
1:A:278:GLN:O	1:A:282:LEU:HD13	1.91	0.69
2:B:6:GLU:O	2:B:7:THR:HG23	1.92	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:466:VAL:O	1:A:467:VAL:HG23	1.94	0.68
1:A:50:ILE:CD1	1:A:52:PRO:HD2	2.24	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
1:A:135:ILE:H	1:A:135:ILE:HD12	1.60	0.65
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:161:GLN:O	2:B:165:THR:HG22	1.98	0.63
1:A:306:ASN:O	1:A:310:LEU:HG	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: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:407:GLN:HG2	2:B:393:ILE:HA	1.82	0.61
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.83	0.61
1:A:438:GLU:HB2	1:A:461:ARG:NH1	2.15	0.60
1:A:518:VAL:O	1:A:522:ILE:HG13	2.01	0.60
1:A:18:GLY:CA	1:A:83:ARG:HD2	2.31	0.60
1:A:94:ILE:H	1:A:94:ILE:HD13	1.66	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
1:A:31:ILE:O	1:A:35:VAL:HG23	2.01	0.60
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.82	0.60
1:A:210:LEU:HD21	1:A:215:THR:HA	1.83	0.60
2:B:323:LYS:HB2	2:B:323:LYS:NZ	2.17	0.60
2:B:368:LEU:O	2:B:372:VAL:HG23	2.02	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
1:A:48:SER:HB2	1:A:147:ASN:HD21	1.68	0.58
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.85	0.58
2:B:422:LEU:HG	2:B:426:TRP:CZ2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:58:THR:O	1:A:130:PHE:HB2	2.04	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
1:A:59:PRO:HG2	1:A:76:ASP:HB2	1.86	0.57
2:B:422:LEU:HA	2:B:425:LEU:HD22	1.85	0.57
1:A:376:THR:HG23	1:A:386:THR:HG23	1.85	0.57
1:A:37:ILE:HD11	1:A:71:TRP:O	2.04	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:10:VAL:CG2	2:B:159:ILE:HD11	2.35	0.56
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.88	0.56
2:B:354:TYR:OH	2:B:357:MET:HG3	2.05	0.56
2:B:376:THR:HG23	2:B:386:THR:HG22	1.86	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
1:A:126:LYS:H	1:A:126:LYS:CD	2.18	0.56
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.41	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
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.36	0.56
2:B:163:SER:HA	2:B:166:LYS:HD3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.89	0.55
1:A:443:ASP:OD1	1:A:444:GLY:N	2.40	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
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.71	0.55
1:A:219:LYS:HD3	1:A:219:LYS:O	2.06	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:402:TRP:CD1	1:A:402:TRP:C	2.80	0.54
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:84:THR:O	1:A:154:LYS:NZ	2.38	0.54
1:A:253:THR:O	1:A:257:ILE:HG13	2.07	0.54
1:A:479:LEU:HD11	1:A:501:TYR:HE2	1.73	0.54
2:B:298:GLU:N	2:B:298:GLU:OE1	2.39	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
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.91	0.53
2:B:369:THR:O	2:B:373:GLN:HG3	2.08	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
1:A:460:ASN:O	1:A:461:ARG:CB	2.57	0.52
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.42	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:363:ASN:HA	1:A:511:ASP:CG	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.44	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
1:A:206:ARG:O	1:A:210:LEU:HD23	2.10	0.52
1:A:51:GLY:N	1:A:52:PRO:HD2	2.24	0.52
1:A:540:LYS:C	1:A:542:ILE:H	2.13	0.51
1:A:210:LEU:HD22	1:A:214:LEU:O	2.10	0.51
2:B:191:SER:CB	2:B:193:LEU:HD13	2.39	0.51
1:A:37:ILE:HD13	1:A:72:ARG:NH1	2.26	0.51
2:B:179:VAL:O	2:B:189:VAL:HA	2.11	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
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
2:B:355:ALA:O	2:B:356:ARG:HG3	2.10	0.51
1:A:226:PRO:HA	1:A:234:LEU:O	2.11	0.51
1:A:253:THR:HA	1:A:291:GLU:O	2.10	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:162:SER:O	2:B:165:THR:HG23	2.11	0.50
2:B:170:PRO:O	2:B:174:GLN:HG3	2.10	0.50
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.41	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:N	1:A:63:ILE:HD12	2.27	0.50
1:A:385:LYS:HB3	1:A:385:LYS:NZ	2.27	0.50
2:B:169:GLU:HG2	2:B:173:LYS:HZ3	1.77	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
2:B:239:TRP:CE3	2:B:378:GLU:HG3	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:225:PRO:HG3	1:A:227:PHE:CZ	2.49	0.48
1:A:474:ASN:O	1:A:478:GLU:HG2	2.14	0.48
2:B:87:PHE:CE2	2:B:155:GLY:HA2	2.48	0.48
1:A:138:GLU:HG2	1:A:138:GLU:O	2.14	0.48
1:A:229:TRP:CD1	1:A:230:MET:HG2	2.49	0.48
1:A:20:LYS:HB3	1:A:21:VAL:H	1.51	0.48
1:A:111:VAL:HG21	1:A:160:PHE:HZ	1.78	0.48
1:A:19:PRO:O	1:A:20:LYS:HG3	2.14	0.48
1:A:94:ILE:HG13	1:A:230:MET:HE2	1.95	0.48
1:A:466:VAL:O	1:A:467:VAL:CG2	2.61	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:421:PRO:HG3	4:A:1025:HOH:O	2.15	0.47
1:A:479:LEU:HD11	1:A:501:TYR:CE2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:194:GLU:HG3	1:A:197:GLN:HB2	1.97	0.47
2:B:195:ILE:HG23	2:B:196:GLY:N	2.30	0.47
1:A:149:LEU:HG	1:A:156:SER:HA	1.97	0.47
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.97	0.47
2:B:278:GLN:OE1	2:B:278:GLN:HA	2.15	0.47
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:368:LEU:HD12	1:A:423:VAL:HG21	1.96	0.46
1:A:466:VAL:HG21	1:A:551:LEU:HB3	1.96	0.46
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.98	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: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:180:ILE:HA	2:B:188:TYR:O	2.16	0.46
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.51	0.46
2:B:350:LYS:HB3	2:B:350:LYS:HE3	1.73	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:11:LYS:O	1:A:85:GLN:HB3	2.16	0.45
1:A:357:MET:N	4:A:1063:HOH:O	2.49	0.45
1:A:319:TYR:OH	1:A:385:LYS:HD3	2.16	0.45
1:A:468:THR:C	1:A:469:LEU:HD23	2.37	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: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
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.52	0.45
1:A:438:GLU:CD	1:A:461:ARG:HD2	2.37	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:356:ARG:HH11	2:B:356:ARG:CG	2.30	0.45
1:A:519:ASN:O	1:A:523:GLU:HG2	2.17	0.45
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.98	0.45
1:A:546:GLU:O	1:A:550:LYS:HG3	2.17	0.45
1:A:332:GLN:HG2	1:A:332:GLN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.99	0.44
2:B:234:LEU:N	2:B:234:LEU:HD12	2.32	0.44
2:B:97:PRO:C	2:B:99:GLY:N	2.70	0.44
1:A:94:ILE:HG21	1:A:183:TYR:HE2	1.81	0.44
1:A:50:ILE:HG23	1:A:51:GLY:N	2.32	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: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:8:VAL:O	1:A:121:ASP:HB2	2.17	0.44
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.81	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
1:A:346:PHE:CD2	1:A:346:PHE:N	2.83	0.44
2:B:29:GLU:HG2	2:B:71:TRP:CZ2	2.53	0.44
2:B:70:LYS:HG3	2:B:70:LYS:H	1.50	0.44
1:A:21:VAL:O	1:A:21:VAL:HG13	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
1:A:249:LYS:HE3	1:A:249:LYS:HB2	1.84	0.43
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.99	0.43
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.66	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:169:GLU:C	2:B:173:LYS:HD3	2.37	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:156:SER:N	2:B:157:PRO:HD2	2.34	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
1:A:184:MET:HB3	1:A:185:ASP:H	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HD3	1:A:73:LYS:N	2.32	0.43
2:B:101:LYS:HG3	2:B:102:LYS:HG3	2.01	0.43
1:A:111:VAL:HG22	1:A:185:ASP:C	2.37	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
1:A:410:TRP:CG	1:A:411:ILE:N	2.87	0.43
1:A:457:TYR:CE1	1:A:464:GLN:HA	2.54	0.43
2:B:205:LEU:HD13	2:B:209:LEU:HD22	2.00	0.43
2:B:266:TRP:CH2	2:B:426:TRP:HB3	2.53	0.43
1:A:12:LEU:HD11	1:A:127:TYR:CD1	2.54	0.42
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.77	0.42
1:A:393:ILE:HG12	1:A:394:GLN:N	2.34	0.42
1:A:498:ASP:HB2	1:A:538:ALA:HA	2.01	0.42
2:B:387:PRO:HG2	2:B:389:PHE:HE1	1.76	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:102:LYS:O	1:A:103:LYS:HD3	2.19	0.42
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.34	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
2:B:234:LEU:N	2:B:234:LEU:CD1	2.83	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:305:GLU:O	1:A:309:ILE:HG13	2.20	0.42
1:A:69:THR:HG22	1:A:69:THR:O	2.20	0.42
1:A:8:VAL:HG13	2:B:53:GLU:OE1	2.20	0.42
1:A:113:ASP:OD1	1:A:113:ASP:O	2.37	0.41
1:A:282:LEU:HD11	1:A:296:THR:HG23	2.02	0.41
2:B:116:PHE:C	2:B:116:PHE:CD1	2.94	0.41
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
2:B:279:LEU:HD23	2:B:299:ALA:HB1	2.01	0.41
2:B:6:GLU:O	2:B:7:THR:CG2	2.64	0.41
1:A:179:VAL:HG13	4:A:1007:HOH:O	2.19	0.41
1:A:357:MET:HE3	1:A:367:GLN:HE22	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:323:LYS:HZ3	2:B:323:LYS:HB2	1.85	0.41
1:A:32:LYS:HD3	1:A:32:LYS:HA	1.87	0.41
2:B:88:TRP:CE3	2:B:88:TRP:HA	2.55	0.41
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
1:A:545:ASN:O	1:A:549:ASP:HB2	2.20	0.41
2:B:366:LYS:O	2:B:370:GLU:HG3	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:393:ILE:O	2:B:416:PHE:HB3	2.21	0.41
2:B:88:TRP:CE3	2:B:88:TRP:CA	3.03	0.41
1:A:94:ILE:CG2	1:A:183:TYR:HE2	2.33	0.41
1:A:539:HIS:O	1:A:540:LYS:HD2	2.21	0.41
1:A:536:VAL:HG12	2:B:258:GLN:HB3	2.02	0.41
2:B:360:ALA:O	2:B:362:THR:N	2.54	0.41
1:A:438:GLU:CG	1:A:439:THR:N	2.84	0.41
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	0.41
1:A:30:LYS:HE2	1:A:71:TRP:CZ3	2.55	0.40
1:A:546:GLU:CG	1:A:547:GLN:NE2	2.84	0.40
1:A:41:MET:HE3	1:A:73:LYS:HE3	2.03	0.40
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.79	0.40
1:A:131:THR:HG23	1:A:142:ILE:O	2.21	0.40
1:A:120:LEU:HB2	1:A:148:VAL:HA	2.03	0.40
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.50	0.40
2:B:49:LYS:HA	2:B:143:ARG:O	2.22	0.40
2:B:87:PHE:O	2:B:88:TRP:C	2.59	0.40
2:B:97:PRO:HD2	2:B:181:CYS:SG	2.62	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
1:A:412:PRO:O	1:A:413:GLU:C	2.60	0.40
2:B:195:ILE:HG12	2:B:199:ARG:NH2	2.37	0.40
1:A:102:LYS:HG3	1:A:237:ASP:HA	2.04	0.40
2:B:125:ARG:HB3	2:B:145:GLN:NE2	2.36	0.40
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.98	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%)	3	3
2	B	392/440 (89%)	348 (89%)	37 (9%)	7 (2%)	9	16
All	All	938/1000 (94%)	823 (88%)	84 (9%)	31 (3%)	4	5

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

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Mol	Chain	Res	Type
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%)	15	28
2	B	362/400 (90%)	338 (93%)	24 (7%)	18	34
All	All	854/899 (95%)	793 (93%)	61 (7%)	16	31

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CSD	A	280	1	4,7,8	1.55	1 (25%)	2,8,10	4.51	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	280	1	-	1/2/6/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	CA-C	2.77	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	6.14	117.23	105.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

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	2.55	8 (34%)	36,36,36	1.37	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	-	-	0/10/32/32	0/2/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	EFZ	C12-C11	-5.23	1.28	1.48
3	A	999	EFZ	C11-C10	-3.55	1.24	1.47
3	A	999	EFZ	C12-C10	-3.54	1.24	1.47
3	A	999	EFZ	C14-N	2.02	1.39	1.35
3	A	999	EFZ	C13-C7	2.18	1.58	1.53
3	A	999	EFZ	C1-N	2.65	1.44	1.39
3	A	999	EFZ	C7-C6	4.37	1.57	1.51
3	A	999	EFZ	C10-C9	6.80	1.70	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	EFZ	C12-C10-C9	-4.79	105.59	119.03
3	A	999	EFZ	C11-C10-C9	-4.77	105.65	119.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	EFZ	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	550/560 (98%)	0.29	45 (8%)	11 11	32, 68, 127, 150	0
2	B	398/440 (90%)	0.19	30 (7%)	14 14	34, 64, 119, 143	0
All	All	948/1000 (94%)	0.25	75 (7%)	12 13	32, 66, 124, 150	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	PRO	7.4
1	A	20	LYS	7.0
2	B	5	ILE	6.2
1	A	67	ASP	6.2
1	A	71	TRP	5.2
2	B	178	ILE	4.9
1	A	69	THR	4.9
2	B	67	ASP	4.9
2	B	357	MET	4.7
1	A	28	GLU	4.6
1	A	66	LYS	4.5
1	A	29	GLU	4.3
1	A	22	LYS	4.2
1	A	68	SER	4.2
1	A	448	ARG	4.1
1	A	65	LYS	4.1
2	B	213	GLY	4.0
2	B	195	ILE	3.9
1	A	92	LEU	3.9
1	A	132	ILE	3.8
1	A	245	VAL	3.8
2	B	88	TRP	3.8
1	A	54	ASN	3.7
1	A	52	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	74	LEU	3.6
1	A	63	ILE	3.5
1	A	24	TRP	3.4
2	B	66	LYS	3.4
1	A	26	LEU	3.4
1	A	554	ALA	3.3
1	A	61	PHE	3.3
2	B	361	HIS	3.1
2	B	69	THR	3.0
1	A	72	ARG	3.0
1	A	130	PHE	3.0
1	A	51	GLY	2.9
1	A	3	SER	2.9
2	B	212	TRP	2.9
2	B	354	TYR	2.8
2	B	183	TYR	2.8
1	A	56	TYR	2.7
2	B	87	PHE	2.7
2	B	177	ASP	2.7
1	A	452	LEU	2.7
1	A	21	VAL	2.7
1	A	43	LYS	2.7
2	B	96	HIS	2.7
1	A	136	ASN	2.6
1	A	138	GLU	2.6
1	A	550	LYS	2.6
1	A	53	GLU	2.5
1	A	73	LYS	2.5
2	B	201	LYS	2.5
2	B	184	MET	2.4
2	B	197	GLN	2.4
2	B	202	ILE	2.4
2	B	43	LYS	2.3
2	B	65	LYS	2.3
2	B	200	THR	2.3
1	A	64	LYS	2.3
1	A	116	PHE	2.3
1	A	469	LEU	2.3
1	A	451	LYS	2.2
2	B	104	LYS	2.2
1	A	62	ALA	2.2
2	B	198	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	70	LYS	2.2
2	B	102	LYS	2.1
1	A	33	ALA	2.1
1	A	244	ILE	2.1
2	B	199	ARG	2.1
1	A	60	VAL	2.1
2	B	410	TRP	2.1
1	A	484	LEU	2.0
2	B	152	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSD	A	280	8/9	0.95	0.14	59,61,78,82	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EFZ	A	999	21/21	0.96	0.14	31,55,65,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.