



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TV6  
Title : HIV-1 Reverse Transcriptase Complexed with CP-94,707  
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Deposited on : 2004-06-28  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

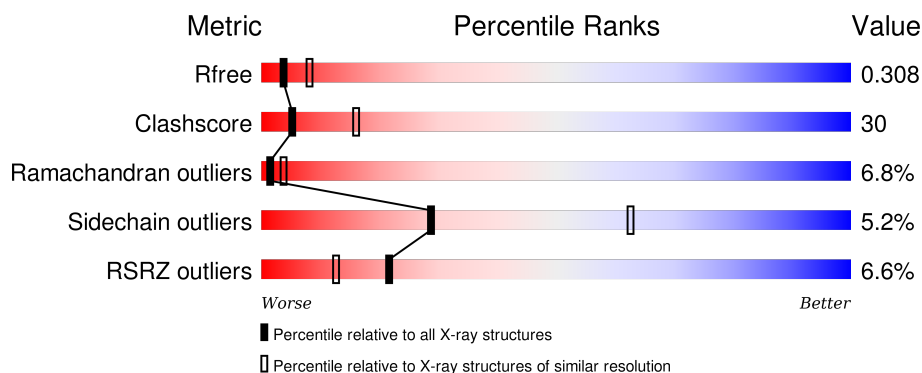
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	<div> <div>5%</div> <div>41%</div> <div>47%</div> <div>7%</div> <div>.</div> </div>
2	B	440	<div> <div>8%</div> <div>45%</div> <div>43%</div> <div>5%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7786 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.

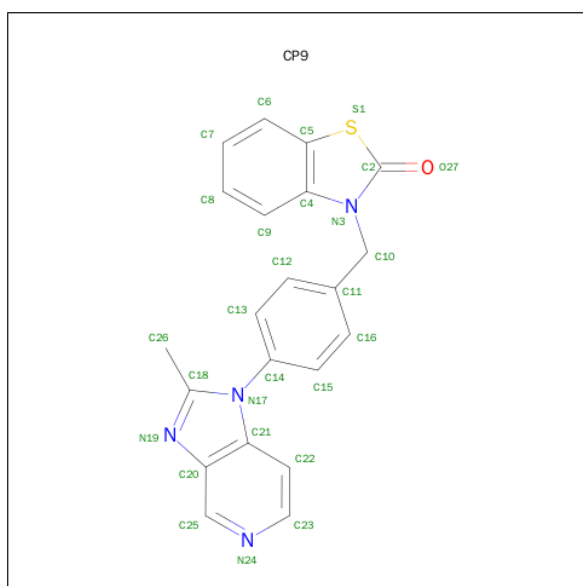
- Molecule 1 is a protein called reverse transcriptase p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4367	2832	722	805	8			

- Molecule 2 is a protein called reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	411	Total	C	N	O	S	0	0	0
			3392	2205	562	618	7			

- Molecule 3 is 3-[4-(2-METHYL-IMIDAZO[4,5-C]PYRIDIN-1-YL)BENZYL]-3H-BENZOTHIADIAZOL-2-ONE (three-letter code: CP9) (formula: C<sub>21</sub>H<sub>16</sub>N<sub>4</sub>OS).

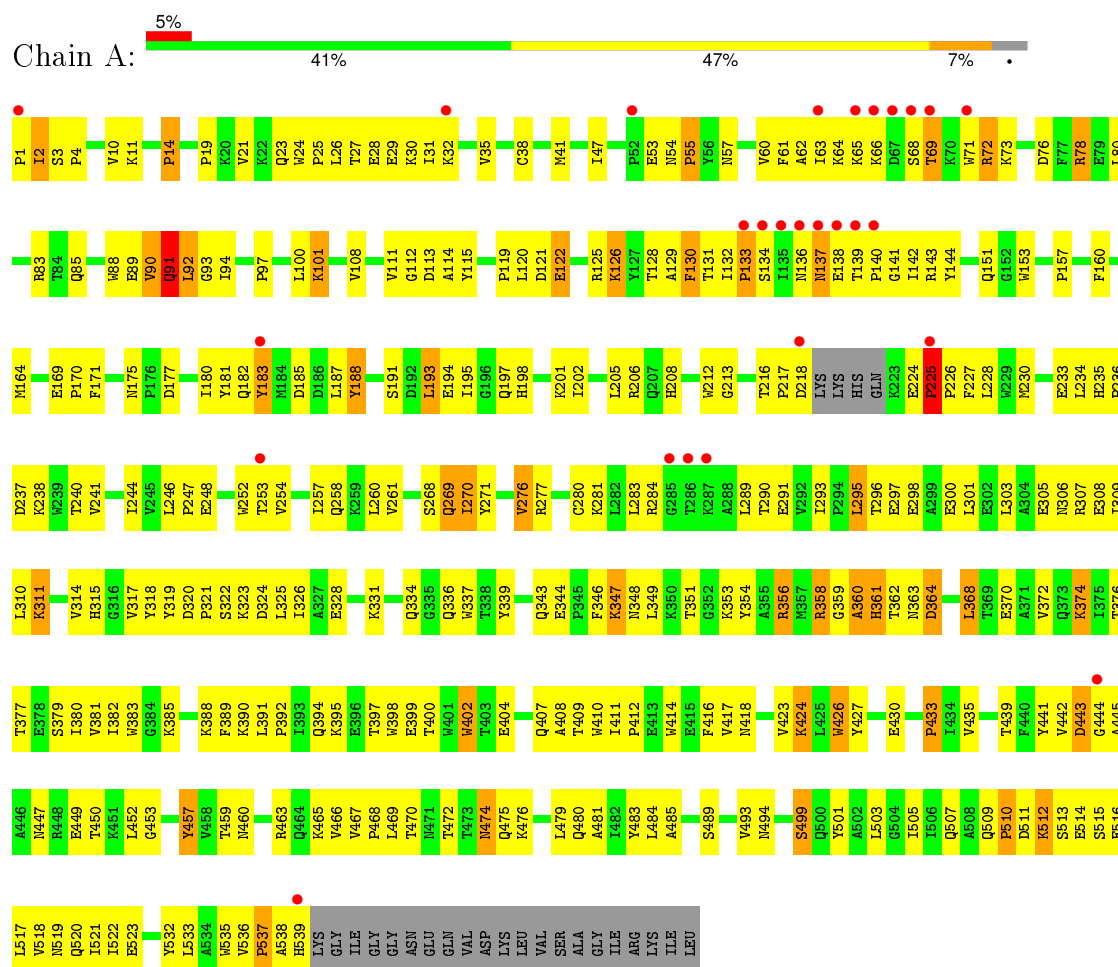


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	21	4	1	1		

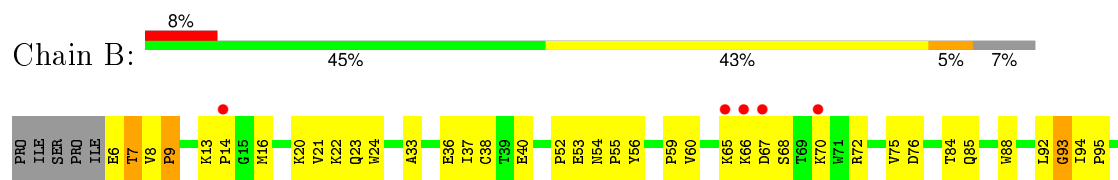
### 3 Residue-property plots

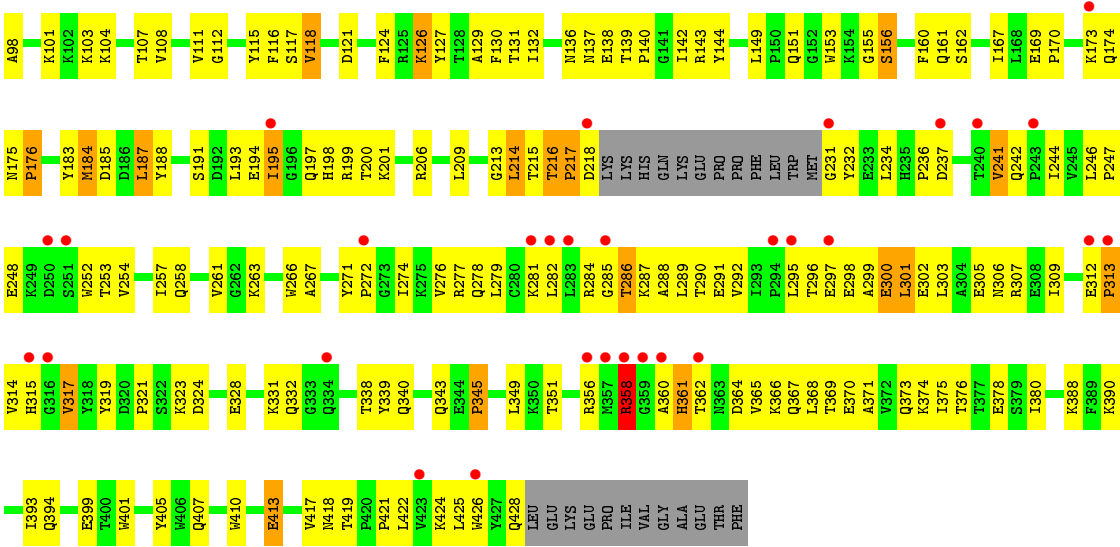
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: reverse transcriptase p66 subunit



#### • Molecule 2: reverse transcriptase p51 subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.91Å 69.04Å 104.33Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.00-2.80) 94.5 (29.52-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.262 , 0.312 0.262 , 0.308	Depositor DCC
$R_{free}$ test set	1995 reflections (5.56%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 66.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 37675 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	7786	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CP9

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	0.43	0/4483	0.70	1/6094 (0.0%)
2	B	0.50	0/3488	0.72	1/4740 (0.0%)
All	All	0.46	0/7971	0.71	2/10834 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	LYS	N-CA-C	6.41	128.30	111.00
2	B	358	ARG	N-CA-C	6.18	127.68	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4367	0	4419	299	0
2	B	3392	0	3418	188	0
3	A	27	0	16	7	0
All	All	7786	0	7853	476	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 30.

All (476) 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:362:THR:HG22	1:A:363:ASN:H	1.12	1.15
2:B:65:LYS:HE3	2:B:72:ARG:HD2	1.24	1.08
1:A:92:LEU:HD23	1:A:93:GLY:H	1.16	1.07
2:B:195:ILE:HG22	2:B:199:ARG:HE	1.19	1.04
1:A:424:LYS:HD2	1:A:426:TRP:HE1	1.22	1.01
1:A:236:PRO:HA	3:A:561:CP9:N24	1.77	0.99
1:A:130:PHE:CE2	1:A:144:TYR:HB2	2.01	0.96
2:B:244:ILE:HD12	2:B:244:ILE:H	1.28	0.95
2:B:241:VAL:HG12	2:B:242:GLN:H	1.28	0.95
1:A:424:LYS:HD2	1:A:426:TRP:NE1	1.82	0.95
1:A:362:THR:HG22	1:A:363:ASN:N	1.87	0.90
1:A:228:LEU:HD23	1:A:228:LEU:H	1.33	0.90
2:B:195:ILE:CG2	2:B:199:ARG:HE	1.86	0.88
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.58	0.86
1:A:28:GLU:O	1:A:32:LYS:HG2	1.75	0.85
1:A:27:THR:HG22	1:A:29:GLU:H	1.38	0.85
1:A:130:PHE:HD2	1:A:130:PHE:H	1.24	0.85
1:A:362:THR:CG2	1:A:363:ASN:H	1.89	0.84
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.18	0.84
1:A:92:LEU:HD23	1:A:93:GLY:N	1.93	0.82
2:B:139:THR:HB	2:B:140:PRO:HD2	1.63	0.81
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.62	0.81
1:A:334:GLN:HE22	1:A:512:LYS:HG3	1.47	0.80
2:B:149:LEU:HB3	2:B:156:SER:OG	1.82	0.79
1:A:193:LEU:HD12	1:A:198:HIS:HA	1.64	0.79
1:A:23:GLN:HE22	1:A:60:VAL:HG23	1.48	0.79
1:A:445:ALA:HA	1:A:474:ASN:ND2	1.98	0.79
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.63	0.78
2:B:213:GLY:O	2:B:215:THR:N	2.16	0.78
2:B:356:ARG:HE	2:B:358:ARG:HG2	1.49	0.78
1:A:459:THR:HG22	1:A:463:ARG:O	1.84	0.78
1:A:424:LYS:HE3	1:A:511:ASP:HB2	1.65	0.77
2:B:126:LYS:HE2	2:B:127:TYR:CZ	2.20	0.76
2:B:232:TYR:HE2	2:B:234:LEU:HD21	1.49	0.76
2:B:324:ASP:O	2:B:343:GLN:HG2	1.87	0.75
1:A:358:ARG:HD3	1:A:358:ARG:H	1.51	0.75
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.67	0.74
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.67	0.74
2:B:281:LYS:HA	2:B:284:ARG:HD3	1.69	0.74
2:B:142:ILE:HD12	2:B:142:ILE:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:GLU:HG2	2:B:390:LYS:HG3	1.70	0.73
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.70	0.72
1:A:519:ASN:O	1:A:523:GLU:HG2	1.88	0.72
1:A:317:VAL:HG12	1:A:348:ASN:O	1.89	0.72
2:B:252:TRP:CD1	2:B:295:LEU:HD21	2.24	0.72
2:B:241:VAL:HG12	2:B:242:GLN:N	2.05	0.72
2:B:305:GLU:O	2:B:309:ILE:HG13	1.89	0.72
1:A:459:THR:HG21	1:A:463:ARG:HB3	1.72	0.71
1:A:424:LYS:HZ1	1:A:511:ASP:HB3	1.56	0.70
2:B:279:LEU:HD23	2:B:282:LEU:HD12	1.73	0.70
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.26	0.70
1:A:30:LYS:HG2	1:A:71:TRP:CZ3	2.27	0.70
1:A:253:THR:HB	1:A:290:THR:HA	1.74	0.70
3:A:561:CP9:H13	3:A:561:CP9:H22	1.73	0.69
2:B:218:ASP:C	2:B:231:GLY:N	2.46	0.69
2:B:195:ILE:HG22	2:B:199:ARG:NE	2.00	0.68
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.73	0.68
1:A:400:THR:O	1:A:404:GLU:HG2	1.94	0.68
1:A:479:LEU:HB3	1:A:517:LEU:HD21	1.76	0.68
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.08	0.68
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.76	0.68
1:A:301:LEU:O	1:A:305:GLU:HG2	1.94	0.67
2:B:303:LEU:O	2:B:307:ARG:HG3	1.95	0.67
1:A:29:GLU:O	1:A:32:LYS:HB2	1.94	0.66
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.29	0.66
1:A:459:THR:CG2	1:A:463:ARG:H	2.09	0.66
1:A:382:ILE:HA	2:B:136:ASN:HD22	1.59	0.66
1:A:134:SER:HB3	1:A:139:THR:O	1.95	0.66
2:B:197:GLN:O	2:B:200:THR:HB	1.96	0.66
2:B:246:LEU:HD12	2:B:307:ARG:HG2	1.78	0.65
1:A:132:ILE:HB	1:A:142:ILE:CG2	2.27	0.65
1:A:445:ALA:HA	1:A:474:ASN:HD21	1.60	0.65
1:A:303:LEU:O	1:A:307:ARG:HG3	1.95	0.65
1:A:424:LYS:HE3	1:A:511:ASP:CB	2.27	0.65
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.78	0.65
1:A:171:PHE:HB2	1:A:208:HIS:CE1	2.31	0.65
1:A:254:VAL:HG13	1:A:283:LEU:HD22	1.78	0.65
1:A:515:SER:O	1:A:517:LEU:N	2.30	0.64
1:A:57:ASN:HA	1:A:129:ALA:O	1.96	0.64
2:B:369:THR:HG22	2:B:373:GLN:NE2	2.12	0.64
2:B:248:GLU:HB2	2:B:307:ARG:NH1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLN:HA	1:A:351:THR:O	1.96	0.64
1:A:364:ASP:OD2	1:A:424:LYS:NZ	2.29	0.64
2:B:214:LEU:O	2:B:216:THR:HG22	1.97	0.64
2:B:244:ILE:CD1	2:B:244:ILE:H	2.06	0.64
1:A:132:ILE:HB	1:A:142:ILE:HG21	1.80	0.63
1:A:226:PRO:HA	1:A:234:LEU:O	1.99	0.63
2:B:242:GLN:HG3	2:B:242:GLN:O	1.96	0.63
1:A:424:LYS:HB2	1:A:426:TRP:NE1	2.14	0.63
1:A:460:ASN:HA	2:B:286:THR:HG22	1.80	0.62
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.99	0.62
1:A:62:ALA:O	1:A:63:ILE:HD13	2.00	0.62
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.82	0.62
1:A:31:ILE:O	1:A:35:VAL:HG23	1.98	0.62
1:A:132:ILE:O	1:A:142:ILE:HB	1.99	0.62
1:A:392:PRO:O	1:A:423:VAL:HG23	1.98	0.62
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.34	0.62
1:A:233:GLU:HB3	1:A:240:THR:HG23	1.81	0.62
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.35	0.61
1:A:1:PRO:HG2	1:A:213:GLY:O	2.01	0.61
2:B:142:ILE:HD12	2:B:142:ILE:N	2.15	0.61
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.35	0.61
1:A:88:TRP:CZ3	2:B:22:LYS:NZ	2.69	0.60
1:A:254:VAL:O	1:A:258:GLN:HG3	2.00	0.60
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.35	0.60
2:B:241:VAL:CG1	2:B:242:GLN:H	2.10	0.60
1:A:171:PHE:HB2	1:A:208:HIS:ND1	2.17	0.60
2:B:13:LYS:O	2:B:16:MET:HB2	2.00	0.60
1:A:235:HIS:CD2	1:A:238:LYS:HE3	2.35	0.60
1:A:424:LYS:CD	1:A:426:TRP:HE1	2.06	0.60
1:A:442:VAL:O	1:A:443:ASP:HB3	2.00	0.60
2:B:33:ALA:O	2:B:36:GLU:HG2	2.02	0.60
1:A:459:THR:CG2	1:A:463:ARG:HB3	2.30	0.60
1:A:130:PHE:N	1:A:130:PHE:CD2	2.69	0.59
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.84	0.59
1:A:130:PHE:N	1:A:130:PHE:HD2	1.97	0.59
2:B:118:VAL:HG22	2:B:149:LEU:HG	1.85	0.59
2:B:115:TYR:HE2	2:B:185:ASP:OD1	1.85	0.59
2:B:232:TYR:CE2	2:B:234:LEU:HD21	2.36	0.59
2:B:314:VAL:HG22	2:B:315:HIS:N	2.18	0.59
1:A:270:ILE:HG23	1:A:271:TYR:CD2	2.38	0.59
2:B:282:LEU:HD21	2:B:296:THR:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.38	0.58
1:A:25:PRO:O	1:A:26:LEU:HD23	2.02	0.58
1:A:88:TRP:HZ3	2:B:22:LYS:NZ	2.02	0.58
1:A:424:LYS:HD2	1:A:426:TRP:CD1	2.37	0.58
1:A:326:ILE:HD13	1:A:388:LYS:HB2	1.84	0.58
2:B:8:VAL:HG12	2:B:8:VAL:O	2.02	0.58
1:A:73:LYS:NZ	1:A:130:PHE:HE1	2.02	0.58
2:B:360:ALA:O	2:B:361:HIS:CG	2.57	0.58
1:A:382:ILE:HG23	2:B:136:ASN:ND2	2.19	0.57
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.86	0.57
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.39	0.57
1:A:427:TYR:OH	1:A:509:GLN:HA	2.04	0.57
2:B:242:GLN:HB3	2:B:351:THR:OG1	2.04	0.57
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.69	0.57
1:A:27:THR:HG22	1:A:29:GLU:N	2.13	0.57
1:A:89:GLU:O	1:A:91:GLN:N	2.38	0.57
1:A:68:SER:O	1:A:69:THR:HG23	2.04	0.57
1:A:252:TRP:CD1	1:A:295:LEU:HD21	2.40	0.57
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.04	0.56
1:A:320:ASP:C	1:A:322:SER:H	2.09	0.56
1:A:334:GLN:HE22	1:A:512:LYS:CG	2.18	0.56
2:B:214:LEU:O	2:B:216:THR:N	2.38	0.56
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.35	0.56
1:A:358:ARG:HD3	1:A:358:ARG:N	2.20	0.56
1:A:2:ILE:HD11	1:A:119:PRO:HB3	1.87	0.56
1:A:535:TRP:CZ3	2:B:422:LEU:HD11	2.40	0.56
2:B:369:THR:HG22	2:B:373:GLN:HE22	1.71	0.56
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.41	0.56
2:B:244:ILE:HD12	2:B:244:ILE:N	2.11	0.56
2:B:248:GLU:HB2	2:B:307:ARG:CZ	2.36	0.56
2:B:366:LYS:HA	2:B:405:TYR:CD2	2.41	0.56
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.35	0.55
2:B:174:GLN:C	2:B:176:PRO:HD3	2.26	0.55
1:A:459:THR:CG2	1:A:463:ARG:N	2.69	0.55
1:A:188:TYR:HB2	3:A:561:CP9:S1	2.46	0.55
1:A:324:ASP:O	1:A:343:GLN:HG2	2.07	0.55
2:B:425:LEU:HD12	2:B:428:GLN:OE1	2.05	0.55
1:A:30:LYS:C	1:A:32:LYS:H	2.08	0.55
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.37	0.55
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.06	0.55
1:A:416:PHE:CD1	1:A:417:VAL:N	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LYS:C	1:A:514:GLU:H	2.09	0.55
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.89	0.54
1:A:112:GLY:C	1:A:114:ALA:H	2.09	0.54
1:A:72:ARG:HD3	1:A:73:LYS:O	2.08	0.54
2:B:92:LEU:O	2:B:93:GLY:O	2.25	0.54
1:A:324:ASP:OD1	1:A:388:LYS:HE3	2.08	0.54
1:A:191:SER:OG	1:A:198:HIS:ND1	2.38	0.54
1:A:260:LEU:HD21	1:A:303:LEU:CD1	2.37	0.54
1:A:281:LYS:O	1:A:284:ARG:HG3	2.06	0.54
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.43	0.54
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.90	0.54
1:A:472:THR:OG1	1:A:476:LYS:HB3	2.08	0.54
2:B:209:LEU:HD12	2:B:217:PRO:HG2	1.90	0.54
2:B:254:VAL:HG21	2:B:288:ALA:O	2.08	0.54
1:A:73:LYS:HZ1	1:A:130:PHE:HE1	1.55	0.54
1:A:489:SER:HB3	1:A:493:VAL:HG22	1.89	0.54
1:A:228:LEU:CD2	1:A:228:LEU:H	2.11	0.54
1:A:28:GLU:O	1:A:28:GLU:HG2	2.07	0.54
1:A:130:PHE:HE2	1:A:144:TYR:HB2	1.67	0.53
1:A:194:GLU:H	1:A:197:GLN:HB3	1.73	0.53
1:A:23:GLN:NE2	1:A:60:VAL:HG23	2.19	0.53
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.24	0.53
1:A:368:LEU:O	1:A:372:VAL:HG23	2.08	0.53
1:A:457:TYR:C	1:A:457:TYR:CD1	2.80	0.53
1:A:30:LYS:C	1:A:32:LYS:N	2.62	0.53
1:A:510:PRO:HG2	1:A:522:ILE:HD11	1.89	0.53
1:A:356:ARG:NE	1:A:359:GLY:HA3	2.23	0.53
1:A:359:GLY:O	1:A:361:HIS:N	2.42	0.53
1:A:296:THR:HG22	1:A:298:GLU:H	1.73	0.53
1:A:511:ASP:OD2	1:A:512:LYS:HG2	2.09	0.53
1:A:30:LYS:HG2	1:A:71:TRP:CH2	2.44	0.53
1:A:395:LYS:HG3	1:A:414:TRP:CH2	2.44	0.53
1:A:447:ASN:OD1	1:A:449:GLU:HB2	2.08	0.53
1:A:100:LEU:HD13	3:A:561:CP9:H16	1.90	0.53
1:A:277:ARG:CB	1:A:336:GLN:NE2	2.73	0.52
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.91	0.52
2:B:115:TYR:C	2:B:117:SER:H	2.13	0.52
1:A:503:LEU:O	1:A:507:GLN:HG3	2.09	0.52
1:A:224:GLU:O	1:A:226:PRO:N	2.42	0.52
2:B:169:GLU:OE1	2:B:173:LYS:HE2	2.08	0.52
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:HG12	1:A:494:ASN:N	2.24	0.52
2:B:7:THR:HG23	2:B:121:ASP:HB2	1.91	0.52
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.75	0.52
2:B:191:SER:OG	2:B:198:HIS:ND1	2.35	0.52
1:A:356:ARG:CZ	1:A:359:GLY:HA3	2.40	0.52
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.91	0.51
1:A:452:LEU:HD23	1:A:470:THR:HA	1.92	0.51
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.93	0.51
2:B:24:TRP:CZ3	2:B:399:GLU:HG2	2.46	0.51
1:A:430:GLU:O	1:A:532:TYR:HD1	1.94	0.51
1:A:111:VAL:HG23	1:A:111:VAL:O	2.10	0.51
3:A:561:CP9:H15	3:A:561:CP9:C26	2.40	0.51
1:A:225:PRO:O	1:A:227:PHE:N	2.40	0.51
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.92	0.51
1:A:108:VAL:HA	1:A:187:LEU:O	2.10	0.51
2:B:94:ILE:HD11	2:B:161:GLN:HG2	1.92	0.51
1:A:320:ASP:O	1:A:322:SER:N	2.44	0.51
2:B:331:LYS:O	2:B:424:LYS:HD2	2.11	0.51
1:A:305:GLU:O	1:A:309:ILE:HG13	2.10	0.51
2:B:76:ASP:OD1	2:B:76:ASP:C	2.48	0.51
1:A:88:TRP:O	1:A:89:GLU:C	2.49	0.51
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.92	0.51
1:A:297:GLU:O	1:A:300:GLU:HG2	2.11	0.51
1:A:424:LYS:HB2	1:A:426:TRP:CD1	2.46	0.51
1:A:180:ILE:O	1:A:181:TYR:HD2	1.94	0.50
2:B:271:TYR:HB2	2:B:274:ILE:HD12	1.94	0.50
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.50	0.50
2:B:194:GLU:O	2:B:195:ILE:C	2.48	0.50
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.92	0.50
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.92	0.50
1:A:112:GLY:O	1:A:114:ALA:N	2.40	0.50
1:A:238:LYS:HD2	1:A:315:HIS:HB3	1.94	0.50
2:B:213:GLY:C	2:B:215:THR:H	2.15	0.50
1:A:362:THR:CG2	1:A:363:ASN:N	2.57	0.50
2:B:365:VAL:HG12	2:B:405:TYR:HE2	1.77	0.50
1:A:489:SER:HB3	1:A:493:VAL:CG2	2.42	0.50
2:B:276:VAL:C	2:B:278:GLN:H	2.14	0.50
1:A:511:ASP:OD2	1:A:512:LYS:N	2.44	0.50
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.45	0.50
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.40	0.50
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG22	1:A:318:TYR:N	2.27	0.49
1:A:276:VAL:O	1:A:276:VAL:HG12	2.12	0.49
2:B:366:LYS:O	2:B:370:GLU:HG3	2.13	0.49
1:A:354:TYR:OH	1:A:370:GLU:OE1	2.25	0.49
1:A:377:THR:O	1:A:381:VAL:HG23	2.13	0.49
1:A:424:LYS:CB	1:A:426:TRP:NE1	2.75	0.49
1:A:136:ASN:O	1:A:138:GLU:N	2.45	0.49
2:B:257:ILE:O	2:B:261:VAL:HG23	2.12	0.49
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.95	0.49
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.48	0.49
1:A:140:PRO:O	1:A:142:ILE:N	2.46	0.49
1:A:217:PRO:O	1:A:218:ASP:O	2.31	0.49
2:B:66:LYS:HE3	2:B:67:ASP:OD1	2.12	0.48
1:A:181:TYR:CE1	2:B:138:GLU:HB3	2.49	0.48
2:B:266:TRP:CD1	2:B:422:LEU:HD12	2.48	0.48
1:A:326:ILE:CD1	1:A:388:LYS:HB2	2.43	0.48
2:B:425:LEU:O	2:B:428:GLN:HG2	2.13	0.48
2:B:254:VAL:O	2:B:258:GLN:HG3	2.12	0.48
1:A:94:ILE:O	1:A:94:ILE:HG13	2.11	0.48
2:B:195:ILE:O	2:B:199:ARG:HD2	2.14	0.48
2:B:136:ASN:O	2:B:137:ASN:HB2	2.12	0.48
2:B:66:LYS:HA	2:B:407:GLN:OE1	2.13	0.48
2:B:13:LYS:HE3	2:B:16:MET:SD	2.54	0.48
1:A:180:ILE:O	1:A:181:TYR:CD2	2.66	0.48
1:A:188:TYR:C	1:A:188:TYR:CD2	2.87	0.48
1:A:62:ALA:C	1:A:63:ILE:HD13	2.34	0.48
2:B:242:GLN:HB3	2:B:351:THR:HG1	1.78	0.48
2:B:7:THR:CG2	2:B:121:ASP:HA	2.44	0.48
1:A:538:ALA:O	1:A:539:HIS:HB2	2.13	0.48
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.49	0.48
1:A:235:HIS:CB	1:A:236:PRO:HD2	2.38	0.48
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.96	0.48
2:B:278:GLN:HE21	2:B:301:LEU:CD2	2.27	0.47
1:A:227:PHE:HD2	1:A:228:LEU:HD23	1.79	0.47
2:B:276:VAL:C	2:B:278:GLN:N	2.67	0.47
2:B:101:LYS:O	2:B:236:PRO:HB2	2.14	0.47
1:A:236:PRO:HA	3:A:561:CP9:C25	2.43	0.47
1:A:459:THR:HG22	1:A:463:ARG:N	2.28	0.47
1:A:90:VAL:CG2	1:A:157:PRO:HB2	2.39	0.47
2:B:115:TYR:O	2:B:117:SER:N	2.48	0.47
2:B:56:TYR:CE2	2:B:126:LYS:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:O	1:A:380:ILE:HG13	2.14	0.47
2:B:72:ARG:NH2	2:B:151:GLN:HE22	2.11	0.47
3:A:561:CP9:C22	3:A:561:CP9:H13	2.44	0.47
1:A:206:ARG:HB3	1:A:206:ARG:CZ	2.44	0.47
1:A:31:ILE:HD13	1:A:133:PRO:HB2	1.96	0.47
2:B:263:LYS:HB3	2:B:426:TRP:CZ3	2.50	0.47
1:A:131:THR:OG1	1:A:143:ARG:HG2	2.14	0.47
1:A:358:ARG:HG2	1:A:360:ALA:H	1.79	0.47
1:A:164:MET:CE	1:A:187:LEU:HD21	2.45	0.47
1:A:198:HIS:O	1:A:202:ILE:HG12	2.15	0.47
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.97	0.47
1:A:202:ILE:O	1:A:206:ARG:HG3	2.15	0.47
2:B:276:VAL:O	2:B:278:GLN:N	2.48	0.47
1:A:19:PRO:CD	1:A:80:LEU:HD13	2.45	0.47
1:A:479:LEU:CB	1:A:517:LEU:HD21	2.45	0.46
1:A:240:THR:OG1	1:A:241:VAL:N	2.48	0.46
1:A:31:ILE:HG22	1:A:31:ILE:O	2.14	0.46
1:A:398:TRP:CZ3	1:A:402:TRP:CD1	3.04	0.46
1:A:60:VAL:C	1:A:61:PHE:HD1	2.18	0.46
1:A:270:ILE:O	1:A:314:VAL:HG11	2.15	0.46
1:A:53:GLU:O	1:A:55:PRO:HD3	2.14	0.46
2:B:101:LYS:O	2:B:236:PRO:CB	2.64	0.46
2:B:94:ILE:HG12	2:B:161:GLN:OE1	2.16	0.46
1:A:90:VAL:O	1:A:91:GLN:C	2.53	0.46
2:B:356:ARG:HD3	2:B:367:GLN:NE2	2.31	0.46
1:A:180:ILE:HA	1:A:188:TYR:O	2.16	0.46
2:B:184:MET:HB3	2:B:185:ASP:H	1.51	0.46
1:A:41:MET:HE2	1:A:47:ILE:HD13	1.98	0.46
1:A:364:ASP:H	1:A:424:LYS:HZ3	1.62	0.46
1:A:358:ARG:HG2	1:A:359:GLY:N	2.31	0.46
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.16	0.46
1:A:417:VAL:O	1:A:417:VAL:HG12	2.15	0.46
1:A:297:GLU:HA	1:A:300:GLU:HG2	1.96	0.46
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.51	0.46
1:A:64:LYS:HD3	1:A:66:LYS:HA	1.98	0.45
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.44	0.45
1:A:270:ILE:HG23	1:A:271:TYR:HD2	1.79	0.45
1:A:10:VAL:HG12	1:A:11:LYS:N	2.31	0.45
1:A:115:TYR:OH	1:A:151:GLN:HB2	2.16	0.45
2:B:388:LYS:HG3	2:B:413:GLU:HB3	1.98	0.45
2:B:115:TYR:CD1	2:B:115:TYR:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:LYS:HB3	2:B:417:VAL:CG1	2.47	0.45
1:A:395:LYS:HA	1:A:414:TRP:CH2	2.49	0.45
1:A:194:GLU:O	1:A:197:GLN:N	2.50	0.45
2:B:267:ALA:HB2	2:B:426:TRP:CZ2	2.51	0.45
2:B:278:GLN:HE21	2:B:301:LEU:HD21	1.81	0.45
2:B:52:PRO:C	2:B:54:ASN:H	2.20	0.45
1:A:257:ILE:O	1:A:261:VAL:HG23	2.17	0.45
2:B:115:TYR:C	2:B:117:SER:N	2.69	0.45
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.97	0.45
1:A:54:ASN:HD21	1:A:126:LYS:HB2	1.81	0.45
1:A:512:LYS:NZ	1:A:523:GLU:OE1	2.48	0.44
1:A:30:LYS:O	1:A:32:LYS:N	2.49	0.44
2:B:213:GLY:C	2:B:215:THR:N	2.70	0.44
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.00	0.44
1:A:68:SER:O	1:A:69:THR:CB	2.65	0.44
2:B:319:TYR:O	2:B:321:PRO:HD3	2.17	0.44
1:A:334:GLN:NE2	1:A:512:LYS:HB2	2.33	0.44
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.52	0.44
1:A:328:GLU:O	1:A:339:TYR:HA	2.17	0.44
2:B:24:TRP:N	2:B:24:TRP:CD1	2.85	0.44
2:B:300:GLU:C	2:B:302:GLU:H	2.20	0.44
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.31	0.44
1:A:3:SER:OG	1:A:4:PRO:HD2	2.17	0.44
1:A:512:LYS:HZ1	1:A:523:GLU:CD	2.20	0.44
1:A:64:LYS:HE3	1:A:69:THR:HA	1.99	0.44
1:A:320:ASP:OD2	1:A:323:LYS:NZ	2.50	0.44
2:B:6:GLU:O	2:B:7:THR:O	2.34	0.44
2:B:312:GLU:HA	2:B:313:PRO:HD2	1.69	0.44
2:B:115:TYR:CE2	2:B:185:ASP:OD1	2.70	0.44
1:A:457:TYR:HD1	1:A:457:TYR:C	2.19	0.44
2:B:160:PHE:O	2:B:161:GLN:C	2.56	0.44
2:B:297:GLU:C	2:B:299:ALA:H	2.20	0.44
1:A:424:LYS:HG3	1:A:424:LYS:O	2.17	0.44
1:A:347:LYS:HA	1:A:347:LYS:HD2	1.61	0.44
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.44
1:A:513:SER:O	1:A:514:GLU:C	2.55	0.44
1:A:193:LEU:HB3	1:A:197:GLN:OE1	2.18	0.44
2:B:104:LYS:HA	2:B:237:ASP:OD1	2.17	0.44
1:A:112:GLY:C	1:A:114:ALA:N	2.70	0.44
2:B:111:VAL:CG1	2:B:187:LEU:HD22	2.46	0.43
2:B:7:THR:HG23	2:B:121:ASP:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.78	0.43
1:A:137:ASN:OD1	1:A:137:ASN:O	2.35	0.43
1:A:518:VAL:O	1:A:522:ILE:HG13	2.18	0.43
1:A:358:ARG:NE	1:A:359:GLY:H	2.16	0.43
1:A:320:ASP:C	1:A:322:SER:N	2.72	0.43
1:A:465:LYS:HG2	1:A:466:VAL:N	2.33	0.43
1:A:374:LYS:O	1:A:374:LYS:HD3	2.18	0.43
1:A:111:VAL:HG22	1:A:185:ASP:O	2.18	0.43
1:A:533:LEU:HA	1:A:533:LEU:HD23	1.80	0.43
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.18	0.43
1:A:331:LYS:HD2	1:A:364:ASP:OD1	2.19	0.43
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.54	0.43
2:B:7:THR:HG23	2:B:121:ASP:HA	2.00	0.43
2:B:60:VAL:HG12	2:B:75:VAL:HG22	2.00	0.43
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.53	0.43
1:A:536:VAL:O	1:A:537:PRO:C	2.57	0.43
1:A:511:ASP:HA	1:A:522:ILE:HD13	2.01	0.43
1:A:475:GLN:NE2	1:A:501:TYR:CZ	2.86	0.43
2:B:314:VAL:CG2	2:B:315:HIS:N	2.81	0.43
1:A:308:GLU:HA	1:A:311:LYS:HG2	2.00	0.43
2:B:112:GLY:CA	2:B:185:ASP:HB3	2.49	0.43
1:A:291:GLU:O	1:A:293:ILE:HG13	2.19	0.43
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.51	0.43
2:B:360:ALA:O	2:B:361:HIS:CD2	2.72	0.43
2:B:393:ILE:HG12	2:B:394:GLN:N	2.33	0.43
2:B:103:LYS:HD3	2:B:103:LYS:HA	1.79	0.43
2:B:390:LYS:HB3	2:B:417:VAL:HG11	2.01	0.43
1:A:76:ASP:OD2	1:A:78:ARG:NH1	2.52	0.43
1:A:459:THR:HG22	1:A:463:ARG:CA	2.49	0.42
2:B:153:TRP:CE2	2:B:155:GLY:HA3	2.54	0.42
2:B:108:VAL:HB	2:B:232:TYR:HB3	2.01	0.42
2:B:279:LEU:CD2	2:B:282:LEU:HD12	2.48	0.42
1:A:296:THR:HG22	1:A:298:GLU:N	2.33	0.42
1:A:453:GLY:O	1:A:469:LEU:HB2	2.20	0.42
2:B:374:LYS:HE2	2:B:378:GLU:CD	2.40	0.42
1:A:424:LYS:NZ	1:A:511:ASP:HB3	2.30	0.42
2:B:194:GLU:O	2:B:197:GLN:N	2.52	0.42
1:A:183:TYR:O	1:A:185:ASP:N	2.52	0.42
2:B:161:GLN:O	2:B:162:SER:C	2.58	0.42
1:A:409:THR:OG1	1:A:410:TRP:N	2.52	0.42
2:B:361:HIS:O	2:B:362:THR:OG1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.82	0.42
1:A:306:ASN:O	1:A:310:LEU:HD13	2.19	0.42
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.44	0.42
1:A:395:LYS:HG3	1:A:414:TRP:CZ2	2.54	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.55	0.42
1:A:469:LEU:HA	1:A:469:LEU:HD23	1.86	0.42
2:B:20:LYS:HE2	2:B:55:PRO:HB2	2.00	0.42
2:B:84:THR:HG21	2:B:124:PHE:HZ	1.84	0.42
1:A:276:VAL:HG12	1:A:280:CYS:HB3	2.01	0.42
1:A:479:LEU:O	1:A:521:ILE:HD11	2.20	0.42
1:A:452:LEU:HD22	1:A:470:THR:HG22	2.01	0.42
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.55	0.42
2:B:70:LYS:HB2	2:B:70:LYS:HE3	1.85	0.42
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.55	0.42
2:B:139:THR:CB	2:B:140:PRO:HD2	2.41	0.42
1:A:501:TYR:CZ	1:A:505:ILE:CD1	3.03	0.41
2:B:371:ALA:O	2:B:375:ILE:HG13	2.18	0.41
1:A:101:LYS:HZ3	1:A:101:LYS:HB2	1.85	0.41
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.55	0.41
1:A:175:ASN:OD1	1:A:201:LYS:NZ	2.45	0.41
1:A:402:TRP:C	1:A:402:TRP:CE3	2.92	0.41
2:B:278:GLN:CG	2:B:299:ALA:HA	2.51	0.41
1:A:379:SER:HA	1:A:383:TRP:CE3	2.55	0.41
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.43	0.41
1:A:23:GLN:HE22	1:A:60:VAL:H	1.68	0.41
1:A:208:HIS:NE2	1:A:212:TRP:NE1	2.63	0.41
1:A:499:SER:OG	1:A:499:SER:O	2.37	0.41
1:A:535:TRP:CH2	2:B:422:LEU:HD11	2.56	0.41
2:B:254:VAL:HG23	2:B:291:GLU:O	2.21	0.41
1:A:164:MET:HE2	1:A:187:LEU:HD21	2.02	0.41
2:B:72:ARG:HH21	2:B:151:GLN:NE2	2.19	0.41
1:A:65:LYS:O	1:A:66:LYS:C	2.58	0.41
1:A:407:GLN:HG2	2:B:393:ILE:HA	2.02	0.41
2:B:126:LYS:HE2	2:B:127:TYR:OH	2.20	0.41
2:B:142:ILE:CD1	2:B:142:ILE:H	2.30	0.41
1:A:27:THR:CG2	1:A:29:GLU:HB3	2.51	0.41
2:B:183:TYR:CD2	2:B:184:MET:HB2	2.56	0.41
2:B:36:GLU:CG	2:B:37:ILE:N	2.84	0.41
1:A:394:GLN:O	1:A:397:THR:N	2.52	0.41
1:A:182:GLN:O	1:A:183:TYR:CD1	2.74	0.41
1:A:126:LYS:O	1:A:128:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:SER:O	1:A:69:THR:CG2	2.69	0.41
2:B:23:GLN:OE1	2:B:60:VAL:HG22	2.20	0.41
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.02	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD3	1.82	0.40
2:B:328:GLU:HG2	2:B:390:LYS:CG	2.47	0.40
1:A:480:GLN:HG2	1:A:517:LEU:HD11	2.03	0.40
2:B:206:ARG:HE	2:B:217:PRO:HD2	1.86	0.40
2:B:278:GLN:HG2	2:B:302:GLU:HB2	2.02	0.40
2:B:167:ILE:O	2:B:167:ILE:HG22	2.20	0.40
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.83	0.40
2:B:339:TYR:C	2:B:340:GLN:NE2	2.74	0.40
2:B:129:ALA:HA	2:B:144:TYR:O	2.21	0.40
1:A:171:PHE:CE2	1:A:205:LEU:HA	2.57	0.40
1:A:268:SER:C	1:A:270:ILE:H	2.24	0.40
1:A:362:THR:O	1:A:510:PRO:HA	2.21	0.40
1:A:444:GLY:O	1:A:445:ALA:HB2	2.22	0.40
1:A:323:LYS:HE2	1:A:344:GLU:OE2	2.21	0.40
2:B:253:THR:O	2:B:257:ILE:HG13	2.21	0.40
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.51	0.40
2:B:107:THR:HA	2:B:232:TYR:O	2.21	0.40
2:B:299:ALA:O	2:B:302:GLU:N	2.55	0.40
1:A:120:LEU:O	1:A:121:ASP:C	2.59	0.40
2:B:284:ARG:O	2:B:287:LYS:HD2	2.22	0.40
1:A:276:VAL:O	1:A:276:VAL:CG1	2.69	0.40
2:B:365:VAL:HG12	2:B:405:TYR:CE2	2.56	0.40
2:B:253:THR:HA	2:B:292:VAL:HA	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/560 (95%)	442 (83%)	51 (10%)	38 (7%)	1	3
2	B	407/440 (92%)	334 (82%)	47 (12%)	26 (6%)	2	4
All	All	938/1000 (94%)	776 (83%)	98 (10%)	64 (7%)	1	4

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	137	ASN
1	A	141	GLY
1	A	225	PRO
1	A	230	MET
1	A	347	LYS
1	A	360	ALA
1	A	418	ASN
1	A	516	GLU
2	B	7	THR
2	B	93	GLY
2	B	214	LEU
2	B	241	VAL
2	B	313	PRO
2	B	358	ARG
1	A	14	PRO
1	A	85	GLN
1	A	237	ASP
1	A	346	PHE
1	A	426	TRP
1	A	443	ASP
2	B	9	PRO
2	B	285	GLY
2	B	345	PRO
2	B	361	HIS
2	B	421	PRO
1	A	69	THR
1	A	91	GLN
1	A	193	LEU
1	A	195	ILE
1	A	269	GLN
1	A	289	LEU
1	A	295	LEU
1	A	311	LYS
1	A	361	HIS

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Mol	Chain	Res	Type
1	A	412	PRO
2	B	14	PRO
2	B	195	ILE
2	B	217	PRO
2	B	272	PRO
2	B	286	THR
2	B	300	GLU
1	A	55	PRO
1	A	78	ARG
1	A	113	ASP
1	A	270	ILE
1	A	321	PRO
1	A	512	LYS
2	B	116	PHE
2	B	277	ARG
2	B	419	THR
1	A	122	GLU
2	B	98	ALA
2	B	176	PRO
2	B	193	LEU
1	A	90	VAL
1	A	276	VAL
2	B	298	GLU
1	A	510	PRO
1	A	537	PRO
2	B	317	VAL
1	A	21	VAL
1	A	433	PRO
2	B	247	PRO

### 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	480/500 (96%)	453 (94%)	27 (6%)	26	59
2	B	373/400 (93%)	356 (95%)	17 (5%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	853/900 (95%)	809 (95%)	44 (5%)	29	62

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	14	PRO
1	A	24	TRP
1	A	72	ARG
1	A	83	ARG
1	A	91	GLN
1	A	92	LEU
1	A	101	LYS
1	A	126	LYS
1	A	130	PHE
1	A	177	ASP
1	A	183	TYR
1	A	188	TYR
1	A	216	THR
1	A	225	PRO
1	A	244	ILE
1	A	248	GLU
1	A	353	LYS
1	A	356	ARG
1	A	358	ARG
1	A	364	ASP
1	A	368	LEU
1	A	374	LYS
1	A	402	TRP
1	A	457	TYR
1	A	474	ASN
1	A	499	SER
2	B	9	PRO
2	B	40	GLU
2	B	53	GLU
2	B	68	SER
2	B	95	PRO
2	B	118	VAL
2	B	126	LYS
2	B	156	SER
2	B	175	ASN
2	B	184	MET

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Mol	Chain	Res	Type
2	B	187	LEU
2	B	216	THR
2	B	301	LEU
2	B	345	PRO
2	B	368	LEU
2	B	413	GLU
2	B	418	ASN

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	137	ASN
1	A	147	ASN
1	A	182	GLN
1	A	278	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	407	GLN
1	A	474	ASN
1	A	475	GLN
1	A	509	GLN
1	A	520	GLN
2	B	91	GLN
2	B	136	ASN
2	B	147	ASN
2	B	151	GLN
2	B	175	ASN
2	B	278	GLN
2	B	394	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	CP9	A	561	-	26,31,31	2.31	9 (34%)	24,45,45	1.52	3 (12%)

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	CP9	A	561	-	-	0/8/8/8	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	CP9	C7-C6	2.06	1.41	1.36
3	A	561	CP9	C15-C14	2.29	1.42	1.38
3	A	561	CP9	C25-N24	2.38	1.36	1.32
3	A	561	CP9	C5-S1	2.57	1.76	1.74
3	A	561	CP9	C13-C14	2.93	1.43	1.38
3	A	561	CP9	C21-N17	3.22	1.44	1.39
3	A	561	CP9	C22-C23	3.75	1.41	1.36
3	A	561	CP9	C14-N17	4.45	1.52	1.46
3	A	561	CP9	C18-N17	6.34	1.45	1.37

All (3) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	561	CP9	C23-C22-C21	-4.35	115.58	119.64
3	A	561	CP9	C25-C20-C21	-2.99	118.10	121.12
3	A	561	CP9	C15-C14-C13	-2.43	117.43	121.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	CP9	7	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	535/560 (95%)	0.17	27 (5%)	32 21	12, 59, 95, 107	0
2	B	411/440 (93%)	0.12	35 (8%)	13 6	4, 39, 99, 105	0
All	All	946/1000 (94%)	0.15	62 (6%)	22 13	4, 53, 98, 107	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	358	ARG	6.1
2	B	357	MET	5.9
2	B	67	ASP	4.8
2	B	231	GLY	4.3
2	B	283	LEU	4.3
2	B	359	GLY	4.1
2	B	362	THR	4.0
1	A	539	HIS	3.7
1	A	135	ILE	3.7
1	A	286	THR	3.5
1	A	32	LYS	3.4
2	B	312	GLU	3.1
1	A	69	THR	3.0
1	A	134	SER	3.0
1	A	225	PRO	3.0
2	B	272	PRO	3.0
2	B	282	LEU	3.0
1	A	137	ASN	2.9
1	A	133	PRO	2.9
2	B	334	GLN	2.9
2	B	423	VAL	2.9
2	B	66	LYS	2.9
2	B	251	SER	2.9
2	B	294	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	240	THR	2.9
2	B	315	HIS	2.9
2	B	356	ARG	2.8
1	A	52	PRO	2.8
1	A	183	TYR	2.7
1	A	63	ILE	2.7
1	A	68	SER	2.7
1	A	285	GLY	2.7
2	B	285	GLY	2.6
1	A	66	LYS	2.6
1	A	139	THR	2.6
1	A	140	PRO	2.6
1	A	67	ASP	2.5
2	B	218	ASP	2.5
1	A	218	ASP	2.5
1	A	138	GLU	2.4
1	A	136	ASN	2.4
1	A	1	PRO	2.4
2	B	70	LYS	2.4
2	B	297	GLU	2.4
1	A	287	LYS	2.4
2	B	243	PRO	2.3
2	B	237	ASP	2.3
2	B	14	PRO	2.3
2	B	313	PRO	2.3
1	A	444	GLY	2.2
2	B	65	LYS	2.2
2	B	250	ASP	2.2
2	B	295	LEU	2.2
2	B	360	ALA	2.1
2	B	173	LYS	2.1
2	B	281	LYS	2.1
2	B	426	TRP	2.1
1	A	71	TRP	2.1
1	A	65	LYS	2.1
2	B	195	ILE	2.0
1	A	253	THR	2.0
2	B	316	GLY	2.0

## 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 [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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CP9	A	561	27/27	0.86	0.31	0.98	62,68,73,74	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.