



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:16 PM GMT

PDB ID : 1JLB
Title : CRYSTAL STRUCTURE OF Y181C MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH NEVIRAPINE
Authors : Ren, J.; Nichols, C.; Bird, L.; Chamberlain, P.; Weaver, K.; Short, S.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2001-07-16
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

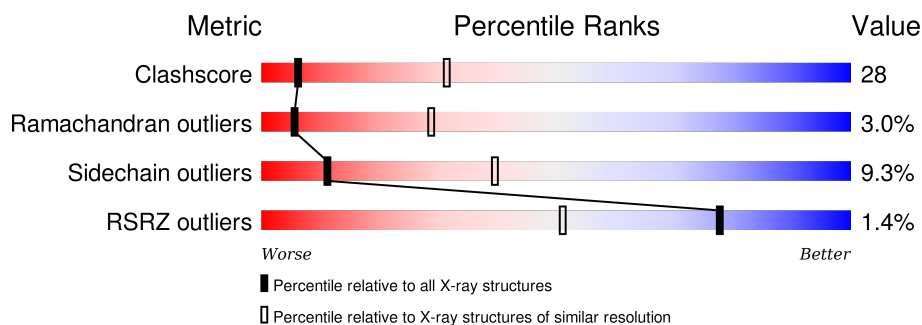
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>2%</div> <div>50%</div> <div>42%</div> <div>6%</div> <div>...</div> </div>
2	B	440	<div> <div>%</div> <div>45%</div> <div>40%</div> <div>7%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NVP	A	999	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7840 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	550	Total	C	N	O	S	0	0	0
			4482	2895	749	829	9			

There are 2 discrepancies between the modelled and reference sequences:

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

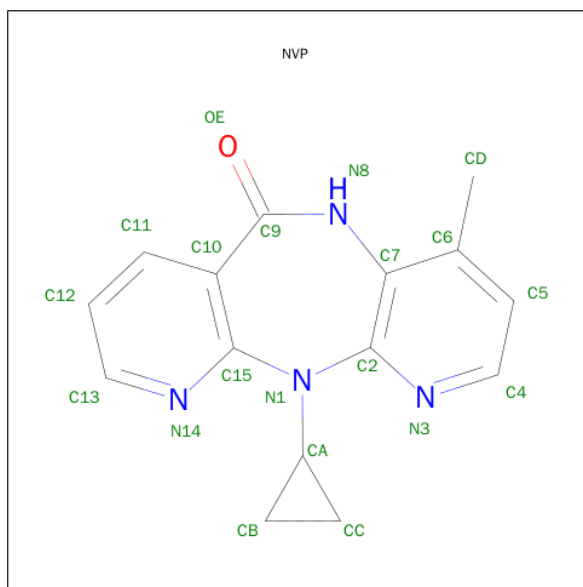
- Molecule 2 is a protein called HIV-1 RT B-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3338	2167	557	606	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 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: C₁₅H₁₄N₄O).

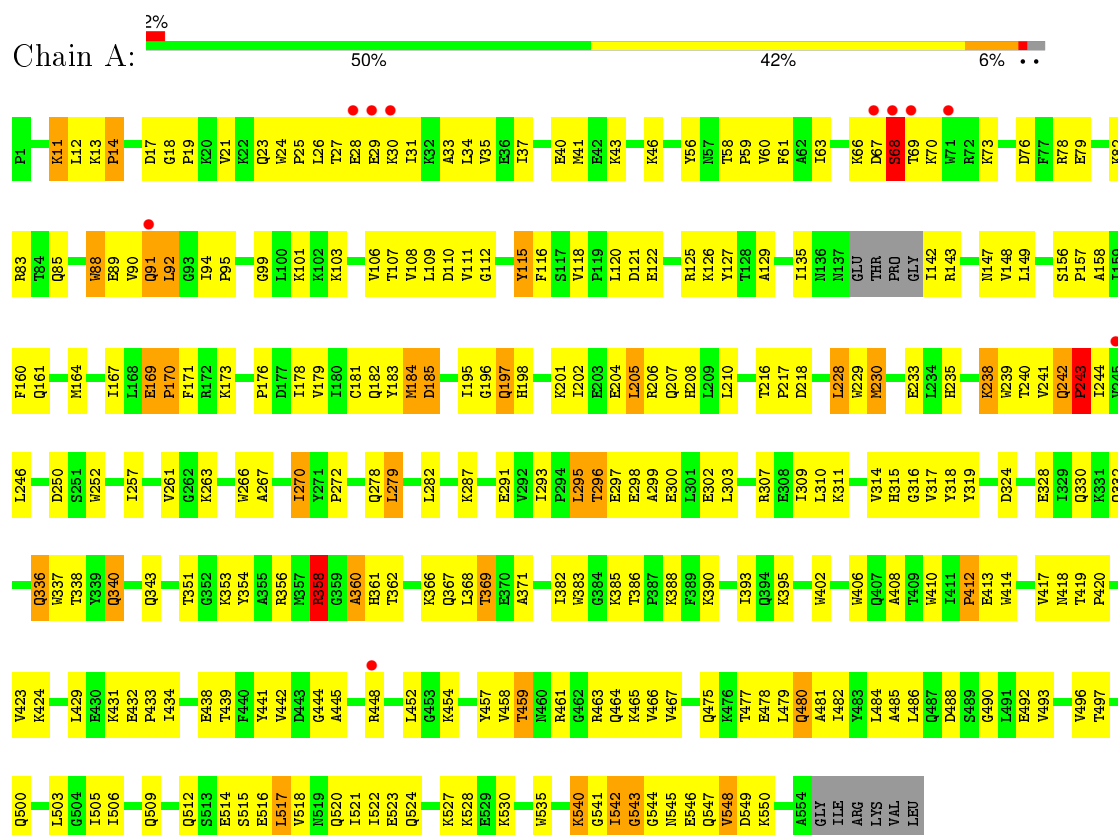


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	4	1		

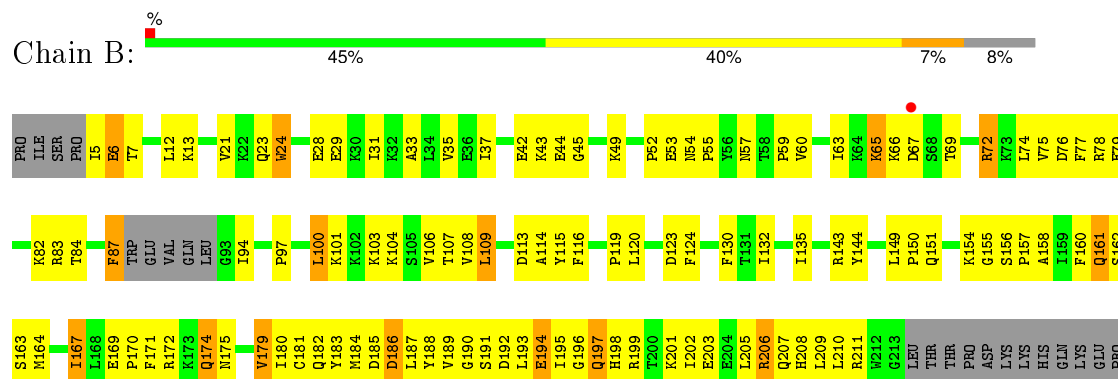
3 Residue-property plots

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: 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, α , β , γ	141.20 Å 110.30 Å 73.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.00 29.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.84-3.00) 97.0 (29.84-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.00 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.251 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 98.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 22844 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7840	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, NVP

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	0.57	0/4588	0.79	1/6231 (0.0%)
2	B	0.54	1/3429 (0.0%)	0.76	0/4653
All	All	0.56	1/8017 (0.0%)	0.77	1/10884 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	181	CYS	CB-SG	6.98	1.94	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	388	LYS	N-CA-C	-5.39	96.44	111.00

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	4482	0	4534	257	0
2	B	3338	0	3374	193	0
3	A	20	0	14	3	0
All	All	7840	0	7922	442	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 (442) 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:358:ARG:HB3	1:A:358:ARG:NH1	1.73	1.04
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	1.96	0.98
1:A:410:TRP:CD1	2:B:363:ASN:HB2	2.00	0.97
2:B:242:GLN:HE21	2:B:242:GLN:HA	1.33	0.92
1:A:79:GLU:HG3	1:A:83:ARG:NH1	1.85	0.91
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.52	0.90
1:A:257:ILE:O	1:A:261:VAL:HG23	1.72	0.90
2:B:72:ARG:HH21	2:B:409:THR:HG22	1.36	0.90
1:A:543:GLY:HA2	1:A:546:GLU:HG2	1.52	0.89
1:A:92:LEU:H	1:A:92:LEU:HD22	1.34	0.88
1:A:23:GLN:HE22	1:A:60:VAL:H	1.20	0.87
1:A:116:PHE:O	1:A:148:VAL:HG21	1.75	0.86
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.10	0.85
1:A:458:VAL:HG12	1:A:548:VAL:HG13	1.60	0.84
2:B:237:ASP:CG	2:B:238:LYS:H	1.80	0.83
2:B:157:PRO:HG2	2:B:184:MET:HA	1.58	0.83
1:A:358:ARG:HH11	1:A:358:ARG:HB3	1.46	0.81
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.41	0.81
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.65	0.78
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.65	0.78
1:A:27:THR:HB	1:A:30:LYS:HG3	1.66	0.78
2:B:247:PRO:HB2	2:B:249:LYS:NZ	1.99	0.78
1:A:270:ILE:HD11	1:A:314:VAL:HG21	1.66	0.77
1:A:90:VAL:O	1:A:91:GLN:HB2	1.85	0.77
1:A:441:TYR:O	1:A:548:VAL:HG21	1.85	0.77
2:B:278:GLN:HB2	2:B:302:GLU:OE2	1.85	0.76
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.67	0.76
1:A:358:ARG:HH22	1:A:512:GLN:HB2	1.50	0.75
1:A:295:LEU:HD23	1:A:299:ALA:HB3	1.69	0.75
2:B:395:LYS:O	2:B:399:GLU:HG2	1.87	0.75
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.68	0.75
1:A:542:ILE:HD12	1:A:542:ILE:H	1.51	0.74
2:B:84:THR:HG22	2:B:154:LYS:HE2	1.68	0.74
1:A:457:TYR:HA	1:A:548:VAL:HG11	1.69	0.74
1:A:37:ILE:O	1:A:40:GLU:HB3	1.86	0.73
1:A:40:GLU:O	1:A:43:LYS:HG2	1.88	0.73
2:B:107:THR:HG23	2:B:232:TYR:HE2	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:ILE:HG22	2:B:6:GLU:H	1.53	0.73
2:B:206:ARG:O	2:B:210:LEU:HD13	1.89	0.72
1:A:545:ASN:O	1:A:549:ASP:HB3	1.89	0.72
1:A:540:LYS:HB3	1:A:542:ILE:CD1	2.20	0.72
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.72	0.72
1:A:244:ILE:CG2	1:A:310:LEU:HD13	2.19	0.72
2:B:94:ILE:HD11	2:B:161:GLN:CD	2.10	0.72
1:A:17:ASP:O	1:A:83:ARG:HD3	1.89	0.71
2:B:421:PRO:O	2:B:425:LEU:HD22	1.90	0.71
1:A:182:GLN:HG2	1:A:183:TYR:N	2.06	0.71
1:A:282:LEU:HD12	1:A:293:ILE:CG2	2.20	0.70
1:A:410:TRP:NE1	2:B:363:ASN:HB2	2.07	0.70
1:A:358:ARG:CZ	1:A:358:ARG:HB3	2.21	0.70
2:B:247:PRO:HB2	2:B:249:LYS:HZ1	1.56	0.70
1:A:417:VAL:HG13	1:A:419:THR:HG22	1.73	0.69
1:A:241:VAL:HG23	1:A:314:VAL:O	1.91	0.69
1:A:356:ARG:HB2	1:A:367:GLN:NE2	2.06	0.69
2:B:100:LEU:HD23	2:B:100:LEU:H	1.56	0.69
2:B:180:ILE:HD11	2:B:189:VAL:HG13	1.75	0.69
1:A:358:ARG:NH2	1:A:512:GLN:HB2	2.08	0.68
1:A:545:ASN:O	1:A:549:ASP:CB	2.41	0.68
2:B:203:GLU:HA	2:B:206:ARG:HD2	1.75	0.68
2:B:174:GLN:HG3	2:B:174:GLN:O	1.94	0.68
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.29	0.68
1:A:169:GLU:O	1:A:173:LYS:HG2	1.92	0.68
1:A:332:GLN:HA	1:A:332:GLN:NE2	2.09	0.68
1:A:111:VAL:HG22	1:A:185:ASP:O	1.95	0.67
1:A:540:LYS:HB3	1:A:542:ILE:HD12	1.77	0.67
1:A:296:THR:HG23	1:A:299:ALA:HB2	1.75	0.67
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.31	0.66
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.78	0.66
1:A:118:VAL:O	1:A:148:VAL:HG23	1.96	0.65
1:A:457:TYR:CA	1:A:548:VAL:HG11	2.26	0.65
2:B:155:GLY:O	2:B:158:ALA:HB3	1.97	0.65
2:B:197:GLN:O	2:B:201:LYS:HB2	1.95	0.65
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.75	0.65
2:B:356:ARG:NH2	2:B:361:HIS:HB3	2.11	0.65
1:A:356:ARG:HB2	1:A:367:GLN:HE22	1.60	0.65
1:A:287:LYS:HG2	1:A:291:GLU:OE2	1.96	0.65
1:A:228:LEU:HD11	1:A:242:GLN:HE22	1.62	0.65
1:A:129:ALA:HB1	1:A:143:ARG:NH2	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ARG:NH2	2:B:409:THR:HG22	2.09	0.65
1:A:517:LEU:O	1:A:520:GLN:HB2	1.96	0.65
1:A:241:VAL:O	1:A:243:PRO:HD3	1.97	0.65
1:A:169:GLU:N	1:A:170:PRO:HD2	2.12	0.64
1:A:332:GLN:HA	1:A:332:GLN:HE21	1.63	0.64
1:A:23:GLN:NE2	1:A:60:VAL:HG12	2.12	0.64
2:B:345:PRO:O	2:B:346:PHE:HB2	1.97	0.64
1:A:356:ARG:CB	1:A:367:GLN:NE2	2.61	0.63
1:A:26:LEU:HD22	1:A:30:LYS:HE2	1.81	0.63
1:A:252:TRP:CD1	1:A:295:LEU:HD12	2.33	0.63
2:B:78:ARG:NH1	2:B:411:ILE:HG22	2.14	0.63
1:A:458:VAL:CG1	1:A:548:VAL:HG13	2.27	0.63
2:B:363:ASN:ND2	2:B:366:LYS:HB2	2.13	0.62
1:A:366:LYS:O	1:A:369:THR:HB	1.99	0.62
2:B:368:LEU:O	2:B:372:VAL:HG23	2.00	0.62
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.30	0.62
1:A:295:LEU:HD23	1:A:299:ALA:CB	2.30	0.61
1:A:122:GLU:CD	1:A:122:GLU:H	2.02	0.61
2:B:100:LEU:H	2:B:100:LEU:CD2	2.13	0.61
2:B:160:PHE:CD1	2:B:160:PHE:O	2.54	0.61
2:B:5:ILE:HG22	2:B:6:GLU:N	2.15	0.61
1:A:27:THR:HG22	1:A:28:GLU:N	2.16	0.61
2:B:66:LYS:HG3	2:B:67:ASP:OD1	2.01	0.61
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.37	0.60
2:B:242:GLN:NE2	2:B:242:GLN:HA	2.13	0.60
1:A:500:GLN:HA	1:A:500:GLN:OE1	2.00	0.60
1:A:490:GLY:H	1:A:528:LYS:NZ	1.99	0.60
2:B:180:ILE:CD1	2:B:189:VAL:HG13	2.32	0.60
1:A:142:ILE:N	1:A:142:ILE:HD12	2.16	0.60
2:B:380:ILE:O	2:B:384:GLY:N	2.35	0.60
2:B:376:THR:CG2	2:B:386:THR:HG22	2.32	0.59
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.02	0.59
2:B:203:GLU:HA	2:B:206:ARG:CD	2.31	0.59
1:A:228:LEU:HD21	1:A:242:GLN:NE2	2.17	0.59
2:B:281:LYS:O	2:B:284:ARG:HG2	2.01	0.59
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.99	0.59
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.84	0.59
1:A:229:TRP:O	1:A:230:MET:C	2.41	0.58
1:A:465:LYS:HG2	1:A:466:VAL:N	2.19	0.58
2:B:79:GLU:O	2:B:83:ARG:HG3	2.02	0.58
2:B:363:ASN:HD21	2:B:366:LYS:HB2	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.39	0.58
1:A:282:LEU:HD12	1:A:293:ILE:HG21	1.84	0.57
1:A:206:ARG:NH2	1:A:218:ASP:HB3	2.19	0.57
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.39	0.57
1:A:541:GLY:O	1:A:542:ILE:C	2.42	0.57
1:A:296:THR:HG23	1:A:299:ALA:CB	2.34	0.57
1:A:94:ILE:HD11	1:A:183:TYR:HE2	1.70	0.57
1:A:546:GLU:O	1:A:550:LYS:CG	2.53	0.57
1:A:457:TYR:C	1:A:548:VAL:HG11	2.25	0.57
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.86	0.57
1:A:441:TYR:HD2	1:A:544:GLY:HA3	1.68	0.57
2:B:195:ILE:HG23	2:B:196:GLY:N	2.19	0.57
2:B:65:LYS:HZ1	2:B:72:ARG:HE	1.51	0.56
2:B:374:LYS:HA	2:B:374:LYS:HE2	1.87	0.56
1:A:463:ARG:NH1	1:A:488:ASP:O	2.38	0.56
1:A:545:ASN:C	1:A:549:ASP:CB	2.74	0.56
1:A:432:GLU:HB2	1:A:433:PRO:HD2	1.88	0.56
2:B:390:LYS:HE2	2:B:415:GLU:OE2	2.06	0.56
2:B:344:GLU:HB3	2:B:347:LYS:HE3	1.87	0.56
1:A:37:ILE:H	1:A:37:ILE:HD12	1.71	0.56
2:B:206:ARG:C	2:B:210:LEU:HD13	2.24	0.56
2:B:13:LYS:HE2	2:B:82:LYS:O	2.06	0.56
1:A:195:ILE:HG13	1:A:196:GLY:N	2.20	0.56
2:B:132:ILE:N	2:B:132:ILE:HD12	2.20	0.56
1:A:300:GLU:HA	1:A:300:GLU:OE2	2.05	0.56
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.87	0.56
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.71	0.55
2:B:42:GLU:OE1	2:B:49:LYS:HG3	2.06	0.55
2:B:65:LYS:HZ3	2:B:72:ARG:HD3	1.70	0.55
1:A:173:LYS:O	1:A:176:PRO:HD3	2.06	0.55
1:A:317:VAL:HG22	1:A:318:TYR:H	1.71	0.55
2:B:43:LYS:C	2:B:45:GLY:H	2.09	0.55
1:A:68:SER:C	1:A:70:LYS:H	2.09	0.55
2:B:237:ASP:O	2:B:239:TRP:N	2.40	0.55
1:A:270:ILE:HD12	1:A:270:ILE:O	2.07	0.55
2:B:426:TRP:O	2:B:429:LEU:HB2	2.07	0.55
2:B:65:LYS:NZ	2:B:72:ARG:HE	2.04	0.54
1:A:25:PRO:O	1:A:26:LEU:HD23	2.07	0.54
2:B:319:TYR:HE2	2:B:325:LEU:HD13	1.73	0.54
2:B:237:ASP:CG	2:B:238:LYS:N	2.54	0.54
1:A:240:THR:CG2	1:A:241:VAL:N	2.69	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LEU:HD23	2:B:100:LEU:N	2.22	0.54
1:A:244:ILE:HG21	1:A:310:LEU:HD22	1.90	0.54
1:A:118:VAL:C	1:A:148:VAL:HG23	2.28	0.54
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.07	0.54
1:A:205:LEU:O	1:A:208:HIS:HB3	2.07	0.54
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.43	0.54
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.89	0.54
1:A:90:VAL:O	1:A:91:GLN:CB	2.54	0.54
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.38	0.54
2:B:207:GLN:HA	2:B:210:LEU:HD22	1.90	0.54
2:B:158:ALA:O	2:B:161:GLN:HB2	2.08	0.54
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.38	0.54
1:A:197:GLN:HA	1:A:197:GLN:HE21	1.73	0.53
1:A:101:LYS:HA	1:A:319:TYR:O	2.07	0.53
1:A:458:VAL:HG12	1:A:548:VAL:CG1	2.35	0.53
1:A:34:LEU:HD21	1:A:73:LYS:HB2	1.89	0.53
1:A:111:VAL:HG22	1:A:185:ASP:C	2.29	0.53
1:A:454:LYS:HA	1:A:467:VAL:O	2.07	0.53
1:A:239:TRP:CH2	1:A:316:GLY:HA3	2.41	0.53
1:A:358:ARG:CZ	1:A:358:ARG:CB	2.87	0.53
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.90	0.53
2:B:169:GLU:O	2:B:172:ARG:HB2	2.09	0.53
1:A:207:GLN:HA	1:A:210:LEU:HB3	1.91	0.53
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.91	0.53
1:A:505:ILE:O	1:A:509:GLN:N	2.34	0.53
2:B:420:PRO:HB2	2:B:423:VAL:HG13	1.90	0.53
2:B:366:LYS:HG2	2:B:405:TYR:CD2	2.44	0.53
2:B:263:LYS:HE2	2:B:425:LEU:HB3	1.90	0.53
1:A:27:THR:HG22	1:A:29:GLU:H	1.73	0.52
1:A:545:ASN:C	1:A:549:ASP:HB2	2.29	0.52
2:B:205:LEU:C	2:B:205:LEU:HD13	2.30	0.52
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.91	0.52
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.92	0.52
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.39	0.52
2:B:193:LEU:CD1	2:B:193:LEU:H	2.22	0.52
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.40	0.52
1:A:545:ASN:HA	1:A:549:ASP:HB2	1.91	0.52
1:A:118:VAL:O	1:A:148:VAL:CG2	2.58	0.51
1:A:545:ASN:CA	1:A:549:ASP:HB2	2.40	0.51
2:B:103:LYS:HE2	2:B:179:VAL:CG2	2.40	0.51
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:VAL:O	1:A:522:ILE:HG13	2.11	0.51
1:A:37:ILE:H	1:A:37:ILE:CD1	2.22	0.51
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.92	0.51
1:A:235:HIS:N	1:A:235:HIS:CD2	2.79	0.51
1:A:178:ILE:CG2	1:A:179:VAL:N	2.74	0.51
1:A:546:GLU:HG3	1:A:547:GLN:NE2	2.26	0.51
1:A:109:LEU:N	1:A:109:LEU:HD12	2.26	0.51
2:B:182:GLN:HB2	2:B:187:LEU:HD12	1.91	0.51
2:B:242:GLN:HB2	2:B:430:GLU:OE1	2.10	0.50
2:B:179:VAL:O	2:B:180:ILE:HD12	2.11	0.50
1:A:520:GLN:HA	1:A:520:GLN:OE1	2.12	0.50
1:A:360:ALA:HB1	1:A:361:HIS:ND1	2.27	0.50
1:A:244:ILE:CG2	1:A:310:LEU:HD22	2.41	0.50
1:A:24:TRP:CD1	1:A:61:PHE:HE1	2.29	0.50
1:A:328:GLU:HG3	1:A:390:LYS:CB	2.40	0.50
2:B:7:THR:CG2	2:B:119:PRO:HG2	2.39	0.50
1:A:115:TYR:O	1:A:149:LEU:HB2	2.12	0.50
1:A:418:ASN:O	1:A:420:PRO:HD3	2.12	0.50
1:A:31:ILE:O	1:A:35:VAL:HG23	2.12	0.50
2:B:266:TRP:CZ3	2:B:426:TRP:CG	2.99	0.50
1:A:92:LEU:H	1:A:92:LEU:CD2	2.11	0.50
1:A:78:ARG:O	1:A:82:LYS:HG3	2.12	0.50
1:A:270:ILE:O	1:A:272:PRO:HD3	2.11	0.49
1:A:235:HIS:ND1	1:A:238:LYS:HE3	2.27	0.49
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.12	0.49
2:B:206:ARG:HH11	2:B:206:ARG:HB3	1.77	0.49
1:A:266:TRP:CE3	1:A:266:TRP:C	2.85	0.49
2:B:366:LYS:O	2:B:370:GLU:HG3	2.12	0.49
1:A:356:ARG:HH22	1:A:371:ALA:HB2	1.77	0.49
2:B:358:ARG:CD	2:B:358:ARG:H	2.24	0.49
2:B:65:LYS:NZ	2:B:72:ARG:HD3	2.28	0.49
2:B:248:GLU:O	2:B:249:LYS:HD3	2.13	0.49
1:A:37:ILE:HD12	1:A:37:ILE:N	2.26	0.49
2:B:361:HIS:HD2	2:B:362:THR:HG23	1.76	0.49
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.47	0.49
2:B:195:ILE:CG2	2:B:196:GLY:N	2.76	0.49
1:A:448:ARG:HH11	1:A:448:ARG:HG2	1.78	0.49
2:B:179:VAL:HG23	2:B:190:GLY:O	2.12	0.49
2:B:183:TYR:HB3	2:B:188:TYR:HE1	1.78	0.48
1:A:116:PHE:C	1:A:148:VAL:HG21	2.33	0.48
2:B:361:HIS:HD2	2:B:362:THR:CG2	2.26	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.59	0.48
2:B:75:VAL:HG12	2:B:76:ASP:N	2.29	0.48
1:A:490:GLY:H	1:A:528:LYS:HZ1	1.60	0.48
1:A:181:CYS:SG	3:A:999:NVP:C4	3.02	0.48
2:B:113:ASP:O	2:B:114:ALA:C	2.52	0.48
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.96	0.48
1:A:33:ALA:O	1:A:37:ILE:HD13	2.13	0.48
2:B:109:LEU:O	2:B:186:ASP:HA	2.14	0.47
1:A:324:ASP:OD2	1:A:324:ASP:N	2.47	0.47
1:A:228:LEU:HD22	1:A:228:LEU:HA	1.69	0.47
1:A:438:GLU:CG	1:A:461:ARG:HD2	2.44	0.47
1:A:478:GLU:O	1:A:481:ALA:HB3	2.14	0.47
1:A:110:ASP:O	1:A:217:PRO:HD3	2.14	0.47
2:B:78:ARG:O	2:B:82:LYS:HG3	2.15	0.47
1:A:120:LEU:HD12	1:A:121:ASP:H	1.79	0.47
2:B:94:ILE:HD11	2:B:161:GLN:CG	2.45	0.47
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.49	0.47
1:A:12:LEU:HD22	1:A:83:ARG:HB3	1.97	0.47
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.96	0.47
2:B:101:LYS:HB2	2:B:101:LYS:HE3	1.63	0.47
1:A:110:ASP:O	1:A:217:PRO:CD	2.63	0.46
1:A:27:THR:CG2	1:A:28:GLU:N	2.78	0.46
2:B:247:PRO:HB2	2:B:249:LYS:HZ2	1.76	0.46
2:B:120:LEU:HD21	2:B:124:PHE:HD2	1.80	0.46
2:B:198:HIS:O	2:B:202:ILE:HG12	2.16	0.46
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.50	0.46
2:B:341:ILE:HD12	2:B:341:ILE:N	2.30	0.46
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.46
1:A:497:THR:O	1:A:535:TRP:HA	2.15	0.46
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.50	0.46
1:A:278:GLN:HG2	1:A:298:GLU:CB	2.42	0.46
2:B:356:ARG:HH11	2:B:356:ARG:HG3	1.80	0.46
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.51	0.46
2:B:358:ARG:H	2:B:358:ARG:HD2	1.80	0.46
1:A:69:THR:HG22	1:A:69:THR:O	2.15	0.46
1:A:23:GLN:HE22	1:A:60:VAL:HG12	1.79	0.46
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.30	0.46
1:A:167:ILE:O	1:A:167:ILE:HG22	2.14	0.46
1:A:106:VAL:HG13	3:A:999:NVP:HCC2	1.98	0.46
2:B:374:LYS:O	2:B:377:THR:HB	2.16	0.46
2:B:132:ILE:HD12	2:B:132:ILE:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.98	0.46
1:A:270:ILE:C	1:A:272:PRO:HD3	2.36	0.46
1:A:445:ALA:N	1:A:477:THR:HG21	2.30	0.46
2:B:376:THR:O	2:B:380:ILE:HG13	2.16	0.45
2:B:205:LEU:O	2:B:208:HIS:HB3	2.17	0.45
1:A:337:TRP:O	1:A:353:LYS:HA	2.16	0.45
1:A:546:GLU:O	1:A:550:LYS:HG3	2.16	0.45
1:A:88:TRP:CE2	1:A:89:GLU:HG3	2.52	0.45
2:B:317:VAL:O	2:B:317:VAL:HG23	2.17	0.45
1:A:26:LEU:HB2	1:A:31:ILE:HG13	1.98	0.45
1:A:99:GLY:HA3	1:A:382:ILE:HG23	1.97	0.45
1:A:11:LYS:NZ	1:A:11:LYS:HB3	2.30	0.45
2:B:106:VAL:HG23	2:B:236:PRO:HG2	1.98	0.45
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.99	0.45
1:A:383:TRP:O	1:A:385:LYS:N	2.50	0.45
2:B:296:THR:HB	2:B:298:GLU:OE2	2.16	0.45
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.51	0.45
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.98	0.45
1:A:434:ILE:HD11	1:A:530:LYS:HB3	1.98	0.45
2:B:167:ILE:O	2:B:208:HIS:NE2	2.47	0.45
1:A:523:GLU:O	1:A:527:LYS:HG2	2.16	0.45
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.82	0.45
2:B:180:ILE:HA	2:B:188:TYR:O	2.17	0.45
2:B:345:PRO:O	2:B:346:PHE:CB	2.65	0.45
2:B:318:TYR:O	2:B:318:TYR:HD2	2.00	0.45
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.52	0.45
1:A:296:THR:O	1:A:299:ALA:HB3	2.17	0.44
1:A:19:PRO:O	1:A:56:TYR:HA	2.16	0.44
1:A:410:TRP:HZ3	2:B:401:TRP:CE2	2.35	0.44
2:B:171:PHE:CG	2:B:205:LEU:HD23	2.53	0.44
2:B:193:LEU:HD12	2:B:193:LEU:N	2.32	0.44
1:A:439:THR:O	1:A:459:THR:HA	2.17	0.44
2:B:103:LYS:HG2	2:B:190:GLY:C	2.38	0.44
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.16	0.44
2:B:31:ILE:O	2:B:35:VAL:HG23	2.18	0.44
2:B:193:LEU:CD1	2:B:193:LEU:N	2.81	0.44
2:B:253:THR:O	2:B:257:ILE:HG12	2.17	0.44
1:A:184:MET:HB3	1:A:185:ASP:H	1.48	0.44
2:B:53:GLU:CD	2:B:53:GLU:H	2.21	0.44
2:B:12:LEU:O	2:B:13:LYS:C	2.56	0.44
1:A:41:MET:HB2	1:A:46:LYS:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TRP:HZ3	2:B:364:ASP:OD2	2.00	0.44
2:B:423:VAL:O	2:B:427:TYR:HD2	2.00	0.44
1:A:412:PRO:O	1:A:413:GLU:C	2.56	0.44
1:A:241:VAL:HG11	1:A:270:ILE:HG12	2.00	0.44
2:B:43:LYS:C	2:B:45:GLY:N	2.70	0.44
1:A:108:VAL:O	1:A:108:VAL:HG13	2.16	0.44
1:A:111:VAL:HG22	1:A:185:ASP:CA	2.48	0.43
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.33	0.43
2:B:303:LEU:HD22	2:B:307:ARG:HE	1.83	0.43
1:A:546:GLU:O	1:A:550:LYS:CB	2.66	0.43
2:B:194:GLU:OE2	2:B:195:ILE:HG22	2.17	0.43
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.53	0.43
1:A:458:VAL:N	1:A:548:VAL:HG11	2.33	0.43
1:A:336:GLN:HA	1:A:354:TYR:O	2.18	0.43
2:B:94:ILE:CG2	2:B:94:ILE:O	2.66	0.43
1:A:317:VAL:HG22	1:A:318:TYR:N	2.32	0.43
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.82	0.43
1:A:340:GLN:HB3	1:A:351:THR:HG22	2.00	0.43
1:A:111:VAL:O	1:A:111:VAL:HG23	2.17	0.43
1:A:178:ILE:HG22	1:A:179:VAL:N	2.33	0.43
1:A:169:GLU:N	1:A:170:PRO:CD	2.80	0.43
1:A:201:LYS:HD3	1:A:201:LYS:HA	1.85	0.43
1:A:13:LYS:HB3	1:A:14:PRO:HD2	2.01	0.43
2:B:360:ALA:HB2	2:B:366:LYS:HD2	1.99	0.43
2:B:179:VAL:O	2:B:189:VAL:HA	2.19	0.43
2:B:209:LEU:O	2:B:210:LEU:C	2.55	0.43
2:B:103:LYS:HD2	2:B:103:LYS:HA	1.77	0.43
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.99	0.43
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.48	0.43
2:B:104:LYS:HB2	2:B:192:ASP:HA	2.00	0.43
2:B:197:GLN:N	2:B:197:GLN:OE1	2.52	0.43
2:B:202:ILE:O	2:B:205:LEU:N	2.52	0.43
1:A:156:SER:N	1:A:157:PRO:CD	2.81	0.43
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.54	0.43
1:A:419:THR:O	1:A:419:THR:HG23	2.19	0.43
2:B:169:GLU:HA	2:B:172:ARG:HB2	2.00	0.43
2:B:77:PHE:O	2:B:78:ARG:C	2.56	0.43
2:B:78:ARG:NH1	2:B:411:ILE:CG2	2.82	0.43
2:B:101:LYS:HE2	2:B:382:ILE:HG23	2.01	0.43
2:B:74:LEU:HD12	2:B:75:VAL:N	2.34	0.43
1:A:324:ASP:O	1:A:343:GLN:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HA	1:A:429:LEU:HD23	1.81	0.42
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.18	0.42
1:A:58:THR:HG23	1:A:76:ASP:O	2.19	0.42
2:B:199:ARG:O	2:B:202:ILE:HB	2.19	0.42
1:A:181:CYS:SG	3:A:999:NVP:HC4	2.59	0.42
1:A:516:GLU:OE2	1:A:516:GLU:HA	2.19	0.42
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.34	0.42
2:B:157:PRO:CG	2:B:184:MET:HA	2.40	0.42
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.48	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.00	0.42
1:A:408:ALA:HB3	2:B:393:ILE:CG1	2.50	0.42
1:A:79:GLU:CG	1:A:83:ARG:HH12	2.24	0.42
1:A:454:LYS:O	1:A:477:THR:CG2	2.67	0.42
1:A:240:THR:HG22	1:A:241:VAL:N	2.34	0.42
1:A:332:GLN:CA	1:A:332:GLN:HE21	2.27	0.42
2:B:201:LYS:HA	2:B:201:LYS:HD2	1.84	0.42
1:A:13:LYS:CB	1:A:14:PRO:HD2	2.50	0.42
1:A:183:TYR:C	1:A:183:TYR:CD1	2.93	0.42
2:B:171:PHE:O	2:B:175:ASN:HB2	2.20	0.42
2:B:206:ARG:O	2:B:209:LEU:N	2.51	0.42
1:A:17:ASP:O	1:A:83:ARG:CD	2.64	0.42
2:B:43:LYS:O	2:B:45:GLY:N	2.53	0.42
1:A:448:ARG:NH1	1:A:448:ARG:HG2	2.34	0.42
2:B:288:ALA:O	2:B:291:GLU:HB3	2.20	0.42
1:A:465:LYS:HG2	1:A:466:VAL:H	1.84	0.41
2:B:236:PRO:HB2	2:B:237:ASP:H	1.64	0.41
1:A:383:TRP:C	1:A:385:LYS:N	2.71	0.41
1:A:90:VAL:HG22	1:A:158:ALA:HB2	2.01	0.41
1:A:66:LYS:O	1:A:67:ASP:HB2	2.20	0.41
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.35	0.41
2:B:356:ARG:CZ	2:B:361:HIS:HB3	2.51	0.41
2:B:163:SER:O	2:B:167:ILE:HG13	2.20	0.41
2:B:326:ILE:O	2:B:341:ILE:HA	2.20	0.41
2:B:33:ALA:O	2:B:37:ILE:HG13	2.20	0.41
1:A:479:LEU:O	1:A:482:ILE:HB	2.20	0.41
1:A:241:VAL:O	1:A:243:PRO:CD	2.67	0.41
1:A:492:GLU:HA	1:A:530:LYS:O	2.21	0.41
2:B:303:LEU:HD22	2:B:307:ARG:NE	2.35	0.41
2:B:295:LEU:HD22	2:B:300:GLU:OE2	2.20	0.41
2:B:170:PRO:O	2:B:174:GLN:HB3	2.20	0.41
1:A:480:GLN:NE2	1:A:484:LEU:HG	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:NZ	2:B:72:ARG:NE	2.69	0.41
2:B:28:GLU:CA	2:B:135:ILE:HD11	2.45	0.41
2:B:376:THR:HG22	2:B:386:THR:HG22	2.01	0.41
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.86	0.41
2:B:195:ILE:HG12	2:B:199:ARG:CZ	2.50	0.41
1:A:201:LYS:O	1:A:204:GLU:HB3	2.20	0.41
2:B:87:PHE:CD1	2:B:87:PHE:N	2.89	0.41
1:A:542:ILE:C	1:A:543:GLY:O	2.58	0.41
2:B:106:VAL:O	2:B:234:LEU:HB2	2.20	0.41
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	0.41
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.56	0.41
1:A:160:PHE:C	1:A:160:PHE:CD1	2.94	0.41
1:A:161:GLN:O	1:A:164:MET:HB3	2.21	0.41
1:A:480:GLN:HE22	1:A:484:LEU:HG	1.85	0.41
2:B:237:ASP:N	2:B:237:ASP:OD1	2.53	0.40
1:A:233:GLU:HB3	1:A:240:THR:HB	2.03	0.40
2:B:78:ARG:HD3	2:B:411:ILE:O	2.21	0.40
2:B:120:LEU:HD12	2:B:150:PRO:HD3	2.01	0.40
2:B:270:ILE:O	2:B:272:PRO:HD3	2.20	0.40
1:A:218:ASP:N	1:A:218:ASP:OD2	2.54	0.40
1:A:457:TYR:HE2	1:A:465:LYS:HD2	1.86	0.40
2:B:103:LYS:HE3	2:B:192:ASP:OD1	2.21	0.40
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.57	0.40
1:A:444:GLY:HA3	1:A:477:THR:HG22	2.03	0.40
2:B:52:PRO:C	2:B:54:ASN:N	2.74	0.40
1:A:541:GLY:O	1:A:546:GLU:HB3	2.21	0.40
2:B:236:PRO:O	2:B:237:ASP:C	2.60	0.40
1:A:242:GLN:O	1:A:242:GLN:HG2	2.21	0.40
1:A:142:ILE:N	1:A:142:ILE:CD1	2.83	0.40
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.56	0.40
1:A:408:ALA:HB3	2:B:393:ILE:HB	2.04	0.40
1:A:546:GLU:HG3	1:A:547:GLN:HE21	1.86	0.40
1:A:282:LEU:HD11	1:A:296:THR:HG22	2.03	0.40
1:A:266:TRP:CE3	1:A:267:ALA:HA	2.56	0.40
2:B:271:TYR:HE1	2:B:312:GLU:O	2.05	0.40
1:A:279:LEU:HB2	1:A:302:GLU:OE1	2.22	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	545/560 (97%)	466 (86%)	60 (11%)	19 (4%)	4	24
2	B	399/440 (91%)	358 (90%)	32 (8%)	9 (2%)	8	36
All	All	944/1000 (94%)	824 (87%)	92 (10%)	28 (3%)	5	29

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	TRP
1	A	91	GLN
1	A	112	GLY
1	A	135	ILE
1	A	542	ILE
2	B	236	PRO
2	B	237	ASP
2	B	238	LYS
1	A	230	MET
1	A	242	GLN
1	A	243	PRO
1	A	358	ARG
1	A	543	GLY
2	B	361	HIS
1	A	85	GLN
1	A	184	MET
2	B	97	PRO
2	B	162	SER
1	A	18	GLY
1	A	238	LYS
1	A	170	PRO
1	A	360	ALA
2	B	44	GLU
2	B	167	ILE
2	B	232	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	68	SER
1	A	14	PRO
1	A	412	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	491/499 (98%)	448 (91%)	43 (9%)	12	42
2	B	367/400 (92%)	330 (90%)	37 (10%)	9	34
All	All	858/899 (95%)	778 (91%)	80 (9%)	11	39

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	63	ILE
1	A	68	SER
1	A	92	LEU
1	A	107	THR
1	A	115	TYR
1	A	169	GLU
1	A	185	ASP
1	A	197	GLN
1	A	205	LEU
1	A	228	LEU
1	A	243	PRO
1	A	250	ASP
1	A	263	LYS
1	A	270	ILE
1	A	279	LEU
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	303	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	309	ILE
1	A	311	LYS
1	A	315	HIS
1	A	336	GLN
1	A	340	GLN
1	A	358	ARG
1	A	362	THR
1	A	368	LEU
1	A	369	THR
1	A	386	THR
1	A	424	LYS
1	A	431	LYS
1	A	452	LEU
1	A	459	THR
1	A	464	GLN
1	A	475	GLN
1	A	480	GLN
1	A	493	VAL
1	A	496	VAL
1	A	514	GLU
1	A	517	LEU
1	A	540	LYS
1	A	548	VAL
2	B	6	GLU
2	B	24	TRP
2	B	29	GLU
2	B	55	PRO
2	B	63	ILE
2	B	65	LYS
2	B	69	THR
2	B	72	ARG
2	B	87	PHE
2	B	100	LEU
2	B	109	LEU
2	B	123	ASP
2	B	161	GLN
2	B	164	MET
2	B	174	GLN
2	B	179	VAL
2	B	186	ASP
2	B	194	GLU
2	B	197	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	206	ARG
2	B	211	ARG
2	B	242	GLN
2	B	276	VAL
2	B	283	LEU
2	B	287	LYS
2	B	289	LEU
2	B	318	TYR
2	B	358	ARG
2	B	361	HIS
2	B	362	THR
2	B	363	ASN
2	B	368	LEU
2	B	379	SER
2	B	418	ASN
2	B	423	VAL
2	B	424	LYS
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	137	ASN
1	A	174	GLN
1	A	197	GLN
1	A	207	GLN
1	A	222	GLN
1	A	242	GLN
1	A	278	GLN
1	A	332	GLN
1	A	336	GLN
1	A	367	GLN
1	A	373	GLN
1	A	475	GLN
1	A	480	GLN
1	A	547	GLN
2	B	57	ASN
2	B	85	GLN
2	B	137	ASN
2	B	151	GLN
2	B	242	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	269	GLN
2	B	361	HIS

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	3,7,8	1.06	0	3,8,10	2.95	2 (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	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	O-C-CA	-2.38	119.30	125.49
1	A	280	CSD	OD1-SG-CB	4.47	112.86	105.40

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 [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NVP	A	999	-	18,23,23	2.70	9 (50%)	18,34,34	1.60	4 (22%)

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	NVP	A	999	-	-	0/0/6/6	0/2/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	NVP	C15-N14	2.31	1.39	1.35
3	A	999	NVP	C2-N3	2.46	1.39	1.35
3	A	999	NVP	C12-C11	3.11	1.43	1.36
3	A	999	NVP	C5-C6	3.17	1.44	1.37
3	A	999	NVP	C12-C13	3.54	1.48	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	NVP	C13-N14	3.65	1.39	1.32
3	A	999	NVP	C4-N3	3.68	1.39	1.32
3	A	999	NVP	C5-C4	3.85	1.46	1.38
3	A	999	NVP	C10-C15	6.03	1.46	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	NVP	CC-CA-N1	-3.15	115.00	118.25
3	A	999	NVP	C4-C5-C6	-3.13	117.73	120.13
3	A	999	NVP	CB-CA-N1	-2.03	116.16	118.25
3	A	999	NVP	C11-C10-C15	2.93	119.74	117.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	NVP	3	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	549/560 (98%)	-0.35	10 (1%) 71 43	31, 83, 140, 150	0
2	B	405/440 (92%)	-0.44	3 (0%) 89 70	38, 77, 131, 150	0
All	All	954/1000 (95%)	-0.39	13 (1%) 78 51	31, 80, 137, 150	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	SER	4.2
1	A	28	GLU	4.0
2	B	232	TYR	3.4
1	A	91	GLN	3.4
2	B	67	ASP	3.3
1	A	67	ASP	3.3
1	A	29	GLU	2.9
1	A	69	THR	2.8
1	A	245	VAL	2.8
2	B	231	GLY	2.4
1	A	71	TRP	2.4
1	A	448	ARG	2.3
1	A	30	LYS	2.1

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. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	CSD	A	280	8/9	0.98	0.10	-	67,70,78,87	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. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NVP	A	999	20/20	0.94	0.28	4.29	57,77,89,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.