



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:45 PM GMT

PDB ID : 1LW0
Title : CRYSTAL STRUCTURE OF T215Y MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH NEVIRAPINE
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Deposited on : 2002-05-30
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
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

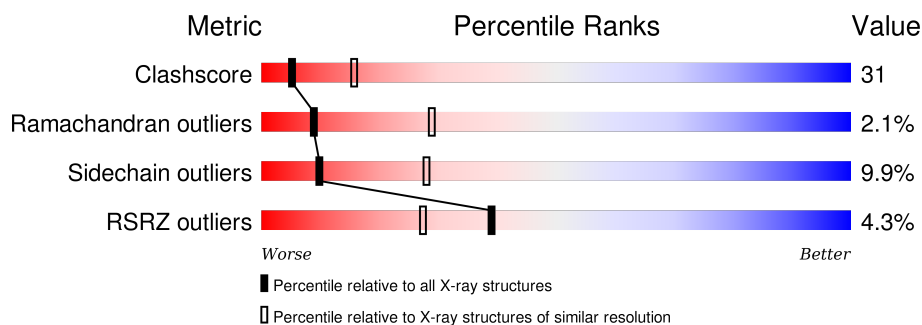
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
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 ≥ 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>3%</div> <div>43%</div> <div>40%</div> <div>8%</div> <div>8%</div> </div>
2	B	440	<div> <div>5%</div> <div>46%</div> <div>41%</div> <div>9%</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	PO4	A	1301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7546 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 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			4210	2730	692	780	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	TYR	THR	ENGINEERED	UNP P04585
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	0	0	0
			3306	2156	546	597	7			

There is a discrepancy between the modelled and reference sequences:

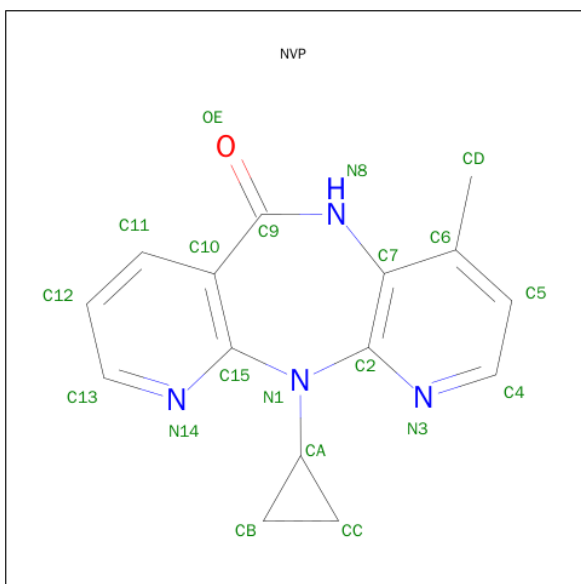
Chain	Residue	Modelled	Actual	Comment	Reference
B	215	TYR	THR	ENGINEERED	UNP P04585

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 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: $C_{15}H_{14}N_4O$).

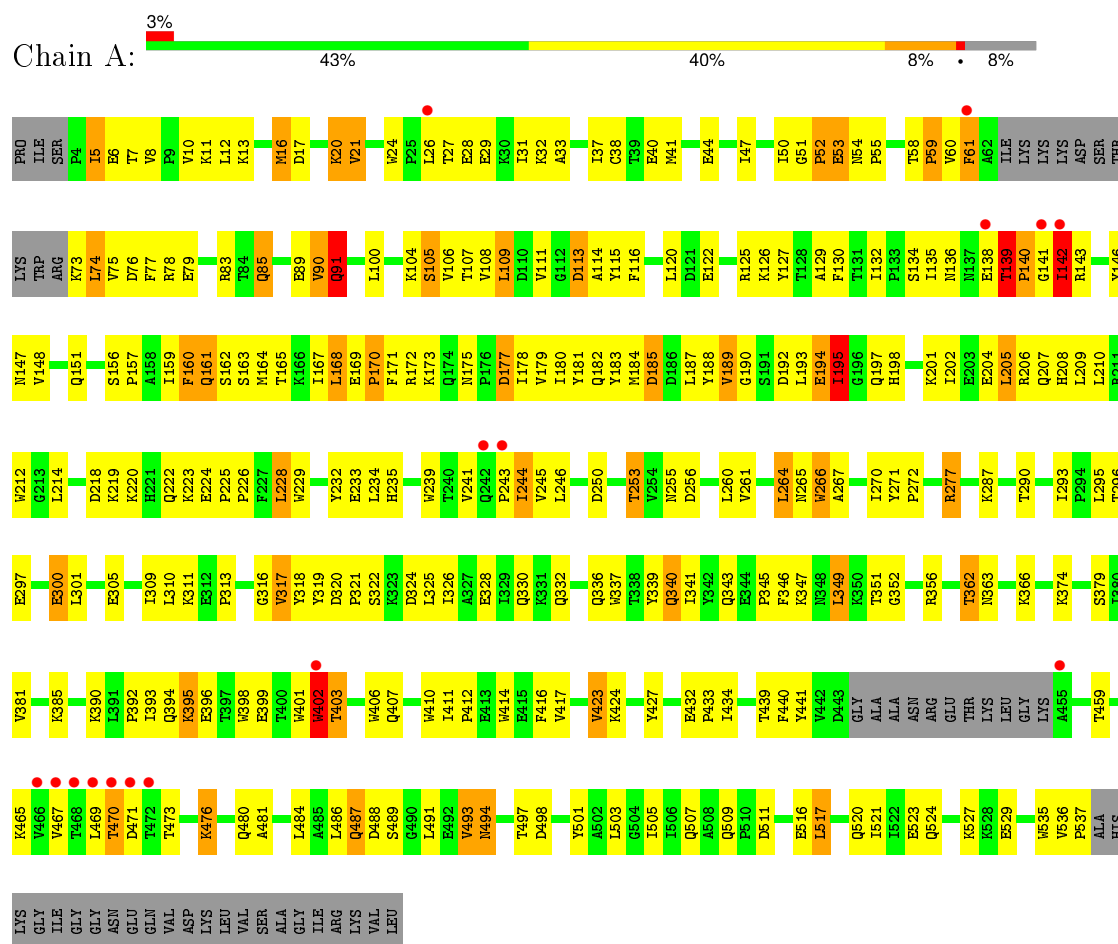


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			20	15	4	1		

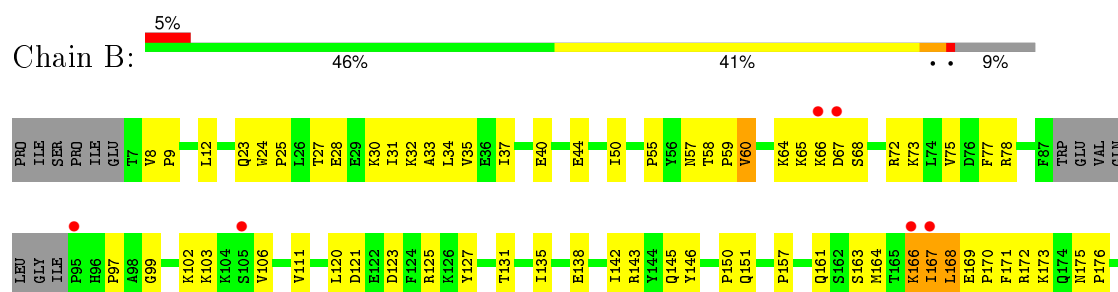
3 Residue-property plots

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 REVERSE TRANSCRIPTASE



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.70 Å 115.00 Å 65.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 2.80 29.85 – 2.78	Depositor EDS
% Data completeness (in resolution range)	93.8 (29.85-2.80) 93.0 (29.85-2.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.80 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.301 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 87.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 25267 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7546	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, PO4, 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	0.59	0/4314	0.77	3/5867 (0.1%)
2	B	0.56	0/3401	0.79	4/4618 (0.1%)
All	All	0.58	0/7715	0.78	7/10485 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	225	PRO	C-N-CD	-10.17	98.23	120.60
2	B	226	PRO	C-N-CA	-6.28	106.00	121.70
2	B	225	PRO	C-N-CA	5.84	146.53	122.00
2	B	227	PHE	N-CA-CB	5.40	120.32	110.60
1	A	349	LEU	N-CA-C	-5.25	96.83	111.00
1	A	494	ASN	N-CA-C	-5.07	97.30	111.00
1	A	228	LEU	CA-CB-CG	-5.04	103.71	115.30

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	4210	0	4230	269	0
2	B	3306	0	3334	199	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	0	2	0
4	A	20	0	14	1	0
All	All	7546	0	7578	463	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 31.

All (463) 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:164:MET:SD	1:A:168:LEU:HD21	1.95	1.06
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.32	1.05
2:B:295:LEU:HD12	2:B:295:LEU:H	1.24	0.99
1:A:395:LYS:HD2	1:A:395:LYS:H	1.25	0.98
1:A:142:ILE:H	1:A:142:ILE:HD13	1.30	0.93
2:B:166:LYS:HA	2:B:166:LYS:HE3	1.50	0.92
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.50	0.92
1:A:28:GLU:OE1	1:A:135:ILE:HG23	1.69	0.91
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.53	0.90
1:A:167:ILE:O	1:A:170:PRO:HD2	1.72	0.89
1:A:195:ILE:H	1:A:195:ILE:HD13	1.37	0.89
1:A:503:LEU:HD12	1:A:535:TRP:HB2	1.54	0.88
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.58	0.86
2:B:168:LEU:HD21	2:B:172:ARG:HD2	1.58	0.85
1:A:277:ARG:NH1	3:A:1301:PO4:O3	2.10	0.84
1:A:89:GLU:C	1:A:91:GLN:H	1.78	0.84
1:A:168:LEU:N	1:A:168:LEU:HD22	1.94	0.83
1:A:395:LYS:HD2	1:A:395:LYS:N	1.93	0.83
2:B:295:LEU:H	2:B:295:LEU:CD1	1.92	0.83
1:A:395:LYS:CD	1:A:395:LYS:H	1.91	0.82
2:B:195:ILE:HD11	2:B:233:GLU:OE1	1.78	0.82
2:B:295:LEU:HD12	2:B:295:LEU:N	1.94	0.82
1:A:317:VAL:HG12	1:A:349:LEU:HD23	1.60	0.82
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.59	0.82
1:A:161:GLN:HA	1:A:182:GLN:HE22	1.45	0.81
2:B:195:ILE:HD11	2:B:233:GLU:CD	2.01	0.80
2:B:206:ARG:NH2	2:B:226:PRO:C	2.35	0.80
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.16	0.80
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.63	0.80
1:A:195:ILE:HD13	1:A:195:ILE:N	1.97	0.79
1:A:139:THR:HB	1:A:140:PRO:HD2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HD12	1:A:6:GLU:H	1.45	0.79
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.65	0.78
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.13	0.78
1:A:138:GLU:HG3	1:A:138:GLU:O	1.84	0.78
1:A:104:LYS:HZ3	1:A:104:LYS:HB3	1.48	0.78
1:A:182:GLN:HA	1:A:187:LEU:HD12	1.66	0.77
2:B:31:ILE:O	2:B:35:VAL:HG23	1.85	0.76
1:A:168:LEU:HD22	1:A:168:LEU:H	1.49	0.76
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.66	0.76
2:B:395:LYS:HD2	2:B:416:PHE:CE1	2.20	0.76
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.21	0.76
1:A:253:THR:HG22	1:A:256:ASP:H	1.52	0.75
1:A:168:LEU:CD2	1:A:168:LEU:H	2.00	0.74
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.16	0.74
2:B:353:LYS:NZ	2:B:428:GLN:HG3	2.02	0.74
1:A:51:GLY:C	1:A:53:GLU:H	1.90	0.73
1:A:503:LEU:CD1	1:A:535:TRP:HB2	2.16	0.73
1:A:89:GLU:OE1	1:A:91:GLN:HA	1.89	0.73
1:A:324:ASP:O	1:A:343:GLN:HG2	1.90	0.71
1:A:27:THR:HG22	1:A:29:GLU:H	1.54	0.71
2:B:66:LYS:HG2	2:B:230:MET:HG2	1.71	0.71
2:B:332:GLN:HB3	2:B:428:GLN:HE22	1.56	0.71
2:B:142:ILE:HD12	2:B:142:ILE:H	1.54	0.70
2:B:206:ARG:NH2	2:B:227:PHE:CD1	2.60	0.70
2:B:28:GLU:CG	2:B:32:LYS:HE3	2.20	0.70
1:A:497:THR:O	1:A:535:TRP:HA	1.92	0.70
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.55	0.70
2:B:203:GLU:O	2:B:206:ARG:HB2	1.92	0.69
1:A:61:PHE:CE2	1:A:74:LEU:HB3	2.28	0.69
1:A:28:GLU:CD	1:A:135:ILE:HG23	2.12	0.69
1:A:28:GLU:O	1:A:32:LYS:HG3	1.93	0.69
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.74	0.68
2:B:420:PRO:O	2:B:423:VAL:HG12	1.93	0.68
2:B:169:GLU:N	2:B:170:PRO:HD2	2.08	0.68
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.08	0.68
1:A:241:VAL:HB	1:A:266:TRP:HE1	1.58	0.68
2:B:275:LYS:HD2	2:B:277:ARG:HH21	1.58	0.68
2:B:175:ASN:N	2:B:176:PRO:HD3	2.09	0.68
1:A:51:GLY:O	1:A:53:GLU:N	2.27	0.67
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.07	0.67
2:B:275:LYS:CD	2:B:277:ARG:HH21	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:HD21	2:B:172:ARG:CD	2.24	0.67
2:B:379:SER:OG	2:B:387:PRO:HG3	1.94	0.67
1:A:363:ASN:HA	1:A:511:ASP:OD1	1.95	0.66
2:B:206:ARG:HH22	2:B:227:PHE:N	1.94	0.66
1:A:104:LYS:NZ	1:A:104:LYS:HB3	2.10	0.66
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.30	0.66
1:A:136:ASN:CB	1:A:139:THR:OG1	2.44	0.65
1:A:208:HIS:O	1:A:212:TRP:CD1	2.49	0.65
2:B:228:LEU:HD11	2:B:409:THR:HG23	1.77	0.65
1:A:168:LEU:N	1:A:168:LEU:CD2	2.59	0.65
1:A:469:LEU:HD11	1:A:480:GLN:HE21	1.62	0.65
2:B:172:ARG:O	2:B:176:PRO:HG3	1.97	0.65
1:A:139:THR:CB	1:A:140:PRO:HD2	2.26	0.65
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.31	0.64
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.33	0.64
1:A:136:ASN:HB3	1:A:139:THR:OG1	1.98	0.64
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.80	0.64
1:A:295:LEU:HD12	1:A:300:GLU:CD	2.18	0.64
1:A:195:ILE:H	1:A:195:ILE:CD1	2.09	0.63
1:A:524:GLN:HA	1:A:524:GLN:OE1	1.97	0.63
1:A:89:GLU:O	1:A:91:GLN:N	2.31	0.63
2:B:266:TRP:O	2:B:269:GLN:HG2	1.99	0.63
2:B:167:ILE:HD12	2:B:212:TRP:CB	2.29	0.62
2:B:175:ASN:ND2	2:B:201:LYS:HD3	2.15	0.62
1:A:244:ILE:HD11	1:A:246:LEU:HD23	1.82	0.62
1:A:89:GLU:C	1:A:91:GLN:N	2.49	0.62
2:B:425:LEU:HD22	2:B:426:TRP:CD1	2.35	0.62
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.81	0.61
1:A:161:GLN:HA	1:A:182:GLN:NE2	2.13	0.61
2:B:206:ARG:HH22	2:B:226:PRO:C	2.02	0.61
2:B:330:GLN:OE1	2:B:340:GLN:NE2	2.28	0.61
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.81	0.61
1:A:392:PRO:O	1:A:423:VAL:HG13	2.02	0.60
2:B:380:ILE:O	2:B:384:GLY:N	2.34	0.60
1:A:239:TRP:O	1:A:316:GLY:N	2.31	0.60
2:B:229:TRP:O	2:B:232:TYR:HB2	2.02	0.59
2:B:311:LYS:O	2:B:312:GLU:HG3	2.03	0.59
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.84	0.59
1:A:467:VAL:HG21	1:A:484:LEU:HD11	1.84	0.58
1:A:245:VAL:HG13	1:A:245:VAL:O	2.03	0.58
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLU:O	2:B:44:GLU:HG3	2.03	0.58
1:A:5:ILE:HD12	1:A:6:GLU:N	2.15	0.58
2:B:135:ILE:O	2:B:138:GLU:HG3	2.03	0.58
1:A:33:ALA:O	1:A:37:ILE:HG13	2.03	0.58
1:A:134:SER:HB2	1:A:140:PRO:O	2.02	0.58
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.38	0.58
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.34	0.58
1:A:398:TRP:NE1	1:A:411:ILE:HD12	2.18	0.58
2:B:167:ILE:HD12	2:B:212:TRP:HB2	1.86	0.57
2:B:395:LYS:HD2	2:B:416:PHE:HE1	1.66	0.57
1:A:125:ARG:HG2	1:A:146:TYR:O	2.05	0.57
1:A:317:VAL:HG12	1:A:349:LEU:CD2	2.34	0.57
1:A:182:GLN:HA	1:A:187:LEU:CD1	2.34	0.57
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.85	0.57
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.35	0.57
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.70	0.57
1:A:175:ASN:HB3	1:A:178:ILE:CG1	2.34	0.56
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.40	0.56
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.05	0.56
1:A:142:ILE:H	1:A:142:ILE:CD1	2.02	0.56
2:B:206:ARG:CZ	2:B:227:PHE:CD1	2.89	0.56
1:A:107:THR:HG22	1:A:109:LEU:HD13	1.88	0.56
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.40	0.56
2:B:276:VAL:HG12	2:B:276:VAL:O	2.05	0.56
2:B:353:LYS:HZ2	2:B:428:GLN:HG3	1.69	0.56
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.06	0.56
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.87	0.56
1:A:115:TYR:CD1	1:A:151:GLN:HG2	2.41	0.56
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.88	0.56
2:B:277:ARG:HG3	2:B:278:GLN:H	1.71	0.56
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.41	0.55
1:A:61:PHE:N	1:A:61:PHE:CD2	2.74	0.55
2:B:325:LEU:O	2:B:387:PRO:HA	2.06	0.55
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.88	0.55
1:A:24:TRP:HZ3	1:A:61:PHE:CG	2.24	0.55
1:A:61:PHE:N	1:A:61:PHE:HD2	2.04	0.55
2:B:28:GLU:HG2	2:B:32:LYS:HE3	1.89	0.55
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.40	0.55
2:B:103:LYS:HE3	2:B:191:SER:HA	1.88	0.55
1:A:8:VAL:HG21	1:A:159:ILE:HG23	1.87	0.55
1:A:10:VAL:HG12	1:A:11:LYS:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:LYS:HA	2:B:405:TYR:CD1	2.42	0.55
2:B:161:GLN:O	2:B:164:MET:HB3	2.06	0.55
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.20	0.55
1:A:108:VAL:HG11	1:A:223:LYS:HB2	1.88	0.55
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.38	0.54
2:B:332:GLN:HB3	2:B:428:GLN:NE2	2.22	0.54
1:A:51:GLY:C	1:A:53:GLU:N	2.59	0.54
1:A:232:TYR:HA	1:A:241:VAL:HA	1.88	0.54
1:A:270:ILE:HG23	1:A:271:TYR:N	2.23	0.54
2:B:173:LYS:HA	2:B:176:PRO:CG	2.33	0.54
2:B:206:ARG:NH2	2:B:227:PHE:N	2.54	0.54
2:B:168:LEU:CD2	2:B:172:ARG:HD2	2.36	0.53
1:A:139:THR:HB	1:A:140:PRO:CD	2.36	0.53
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.40	0.53
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.88	0.53
1:A:346:PHE:CD1	1:A:346:PHE:N	2.76	0.53
1:A:104:LYS:NZ	1:A:104:LYS:CB	2.71	0.53
1:A:516:GLU:O	1:A:520:GLN:HG3	2.07	0.53
2:B:208:HIS:O	2:B:212:TRP:HE3	1.91	0.53
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.08	0.53
1:A:208:HIS:O	1:A:212:TRP:HD1	1.90	0.53
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.43	0.53
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.39	0.53
1:A:160:PHE:O	1:A:161:GLN:C	2.46	0.53
1:A:402:TRP:CG	1:A:403:THR:N	2.77	0.53
1:A:108:VAL:O	1:A:108:VAL:HG13	2.09	0.53
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.44	0.53
1:A:17:ASP:O	1:A:83:ARG:HD3	2.09	0.53
2:B:142:ILE:HD12	2:B:142:ILE:N	2.24	0.52
1:A:207:GLN:NE2	1:A:207:GLN:CA	2.72	0.52
2:B:237:ASP:OD2	2:B:238:LYS:HG3	2.09	0.52
1:A:209:LEU:O	1:A:214:LEU:HB2	2.09	0.52
1:A:37:ILE:O	1:A:41:MET:HG3	2.08	0.52
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.45	0.52
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.90	0.52
2:B:229:TRP:CE3	2:B:229:TRP:HA	2.45	0.52
2:B:106:VAL:O	2:B:233:GLU:HA	2.10	0.52
1:A:253:THR:HB	1:A:256:ASP:OD2	2.10	0.52
1:A:113:ASP:HA	1:A:116:PHE:CD2	2.46	0.52
1:A:139:THR:CB	1:A:140:PRO:CD	2.88	0.51
2:B:371:ALA:O	2:B:375:ILE:HG13	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:SER:O	2:B:167:ILE:HG22	2.10	0.51
1:A:139:THR:HG22	1:A:140:PRO:CD	2.40	0.51
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.92	0.51
2:B:169:GLU:N	2:B:170:PRO:CD	2.73	0.51
1:A:253:THR:HG23	1:A:255:ASN:H	1.75	0.51
2:B:275:LYS:HD2	2:B:277:ARG:NH2	2.24	0.51
1:A:219:LYS:HE3	1:A:224:GLU:OE1	2.10	0.51
1:A:244:ILE:HD13	1:A:244:ILE:C	2.31	0.51
2:B:254:VAL:O	2:B:258:GLN:HG3	2.10	0.51
2:B:167:ILE:HD12	2:B:212:TRP:HB3	1.93	0.51
1:A:523:GLU:O	1:A:527:LYS:HG2	2.11	0.51
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.41	0.51
2:B:241:VAL:HG11	2:B:313:PRO:HG3	1.93	0.51
2:B:335:GLY:O	2:B:355:ALA:HA	2.10	0.51
1:A:100:LEU:HB2	1:A:318:TYR:CD1	2.46	0.50
1:A:8:VAL:HG21	1:A:159:ILE:HG12	1.94	0.50
2:B:206:ARG:CZ	2:B:227:PHE:CE1	2.95	0.50
2:B:28:GLU:HG3	2:B:32:LYS:HE3	1.93	0.50
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.11	0.50
1:A:326:ILE:O	1:A:341:ILE:HA	2.10	0.50
1:A:363:ASN:ND2	1:A:401:TRP:CH2	2.78	0.50
1:A:111:VAL:HG23	1:A:185:ASP:O	2.12	0.50
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.93	0.50
2:B:227:PHE:CD2	2:B:231:GLY:HA2	2.47	0.50
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.45	0.50
1:A:100:LEU:O	1:A:318:TYR:HB3	2.11	0.50
2:B:33:ALA:O	2:B:37:ILE:HG13	2.12	0.50
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.42	0.50
2:B:199:ARG:HH22	2:B:232:TYR:HE2	1.60	0.50
1:A:188:TYR:N	1:A:188:TYR:CD1	2.80	0.50
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.47	0.50
1:A:194:GLU:O	1:A:194:GLU:HG3	2.12	0.50
2:B:206:ARG:NH2	2:B:227:PHE:CG	2.79	0.49
1:A:104:LYS:NZ	1:A:193:LEU:O	2.42	0.49
2:B:28:GLU:CA	2:B:135:ILE:HD11	2.42	0.49
1:A:40:GLU:O	1:A:44:GLU:HG3	2.12	0.49
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.94	0.49
2:B:173:LYS:CA	2:B:176:PRO:HG3	2.35	0.49
2:B:249:LYS:HG3	2:B:252:TRP:CE2	2.47	0.49
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.47	0.49
1:A:277:ARG:NH1	3:A:1301:PO4:P	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD21	1:A:233:GLU:HG3	1.95	0.49
2:B:385:LYS:HG2	2:B:386:THR:N	2.28	0.49
1:A:114:ALA:CB	1:A:185:ASP:OD2	2.61	0.49
1:A:120:LEU:HB2	1:A:148:VAL:O	2.13	0.49
2:B:99:GLY:HA2	2:B:102:LYS:HE2	1.95	0.49
1:A:218:ASP:O	1:A:222:GLN:HG3	2.13	0.48
2:B:316:GLY:O	2:B:318:TYR:CD2	2.65	0.48
2:B:205:LEU:CD2	2:B:209:LEU:HG	2.43	0.48
1:A:113:ASP:O	1:A:114:ALA:C	2.52	0.48
1:A:345:PRO:C	1:A:346:PHE:HD1	2.17	0.48
1:A:340:GLN:HA	1:A:351:THR:HA	1.94	0.48
1:A:104:LYS:HD3	1:A:192:ASP:O	2.14	0.48
1:A:164:MET:O	1:A:168:LEU:HD23	2.14	0.48
1:A:126:LYS:HG3	1:A:127:TYR:N	2.28	0.48
2:B:195:ILE:O	2:B:199:ARG:HG3	2.14	0.48
1:A:164:MET:O	1:A:165:THR:C	2.53	0.48
1:A:164:MET:SD	1:A:168:LEU:CD2	2.87	0.48
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.79	0.48
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.13	0.48
2:B:208:HIS:CD2	2:B:212:TRP:HZ3	2.32	0.47
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.96	0.47
1:A:317:VAL:CG1	1:A:349:LEU:HD23	2.38	0.47
1:A:228:LEU:HA	1:A:232:TYR:O	2.14	0.47
2:B:209:LEU:O	2:B:213:GLY:N	2.47	0.47
1:A:310:LEU:HA	1:A:310:LEU:HD23	1.66	0.47
2:B:353:LYS:HZ3	2:B:428:GLN:HG3	1.77	0.47
1:A:265:ASN:O	1:A:266:TRP:C	2.52	0.47
1:A:481:ALA:O	1:A:484:LEU:HB2	2.13	0.47
2:B:249:LYS:HD3	2:B:251:SER:O	2.13	0.47
1:A:100:LEU:O	1:A:319:TYR:N	2.45	0.47
1:A:427:TYR:OH	1:A:509:GLN:HA	2.14	0.47
1:A:265:ASN:O	1:A:267:ALA:N	2.47	0.47
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.45	0.47
1:A:253:THR:CG2	1:A:255:ASN:H	2.27	0.47
1:A:21:VAL:HG22	1:A:59:PRO:CD	2.44	0.47
1:A:8:VAL:CG2	1:A:159:ILE:HG23	2.45	0.47
1:A:325:LEU:HD22	1:A:341:ILE:CG2	2.45	0.47
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.15	0.47
1:A:305:GLU:O	1:A:309:ILE:HG13	2.15	0.47
1:A:5:ILE:HG13	1:A:6:GLU:O	2.15	0.47
2:B:423:VAL:HG13	2:B:424:LYS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ALA:O	2:B:389:PHE:HA	2.15	0.47
1:A:169:GLU:O	1:A:172:ARG:HB2	2.15	0.47
2:B:195:ILE:HD11	2:B:233:GLU:CG	2.45	0.47
1:A:270:ILE:CG2	1:A:271:TYR:N	2.77	0.47
2:B:28:GLU:O	2:B:32:LYS:HG3	2.15	0.46
1:A:393:ILE:O	1:A:414:TRP:CZ3	2.67	0.46
2:B:170:PRO:HG2	2:B:208:HIS:CE1	2.49	0.46
2:B:306:ASN:O	2:B:310:LEU:HG	2.16	0.46
2:B:40:GLU:O	2:B:40:GLU:HG3	2.15	0.46
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.50	0.46
1:A:177:ASP:OD1	1:A:177:ASP:N	2.42	0.46
1:A:21:VAL:HG22	1:A:59:PRO:CG	2.45	0.46
1:A:195:ILE:CD1	1:A:195:ILE:N	2.66	0.46
2:B:175:ASN:N	2:B:176:PRO:CD	2.79	0.46
2:B:365:VAL:O	2:B:366:LYS:C	2.51	0.46
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.50	0.46
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.16	0.46
1:A:229:TRP:HB3	1:A:234:LEU:HD12	1.98	0.46
2:B:345:PRO:O	2:B:346:PHE:HB2	2.15	0.46
1:A:58:THR:HG21	1:A:77:PHE:CD2	2.50	0.46
1:A:136:ASN:HB2	1:A:139:THR:OG1	2.16	0.45
2:B:428:GLN:O	2:B:428:GLN:HG2	2.16	0.45
1:A:20:LYS:HG3	1:A:55:PRO:O	2.16	0.45
2:B:206:ARG:NH2	2:B:226:PRO:O	2.48	0.45
1:A:439:THR:O	1:A:459:THR:HA	2.15	0.45
1:A:207:GLN:HE21	1:A:207:GLN:CA	2.30	0.45
1:A:229:TRP:HB3	1:A:234:LEU:CD1	2.47	0.45
1:A:201:LYS:O	1:A:204:GLU:HB2	2.17	0.45
1:A:134:SER:HB2	1:A:140:PRO:C	2.36	0.45
2:B:97:PRO:C	2:B:99:GLY:H	2.20	0.45
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.98	0.45
1:A:250:ASP:OD2	1:A:250:ASP:N	2.50	0.45
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.46	0.45
2:B:380:ILE:O	2:B:384:GLY:HA2	2.17	0.45
1:A:332:GLN:HG2	1:A:332:GLN:O	2.16	0.45
2:B:260:LEU:HD23	2:B:279:LEU:HD22	1.98	0.45
2:B:111:VAL:CG1	2:B:187:LEU:HD22	2.34	0.45
1:A:77:PHE:O	1:A:78:ARG:C	2.55	0.45
2:B:317:VAL:HG23	2:B:317:VAL:O	2.16	0.45
1:A:320:ASP:OD2	1:A:322:SER:OG	2.30	0.45
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:O	1:A:417:VAL:HG13	2.17	0.45
2:B:103:LYS:HG2	2:B:191:SER:N	2.32	0.45
1:A:363:ASN:ND2	1:A:401:TRP:CZ3	2.85	0.45
1:A:11:LYS:O	1:A:85:GLN:HG2	2.17	0.45
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.52	0.45
1:A:225:PRO:HA	1:A:226:PRO:C	2.36	0.45
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.52	0.45
2:B:168:LEU:C	2:B:170:PRO:HD2	2.36	0.44
2:B:274:ILE:CD1	2:B:310:LEU:HD21	2.41	0.44
2:B:389:PHE:HB3	2:B:391:LEU:HD21	1.99	0.44
2:B:379:SER:HA	2:B:383:TRP:CE3	2.52	0.44
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.52	0.44
2:B:368:LEU:O	2:B:372:VAL:HG23	2.17	0.44
1:A:13:LYS:O	1:A:16:MET:HB2	2.18	0.44
1:A:61:PHE:CZ	1:A:74:LEU:HD23	2.53	0.44
2:B:379:SER:HB3	2:B:385:LYS:O	2.17	0.44
2:B:319:TYR:O	2:B:321:PRO:HD3	2.18	0.44
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.52	0.44
1:A:476:LYS:HD2	1:A:476:LYS:O	2.17	0.44
2:B:241:VAL:HG13	2:B:351:THR:OG1	2.17	0.44
1:A:201:LYS:HD3	1:A:204:GLU:CD	2.38	0.44
2:B:34:LEU:HD21	2:B:73:LYS:HG3	1.99	0.44
2:B:78:ARG:NH2	2:B:411:ILE:HG21	2.33	0.44
1:A:467:VAL:CG2	1:A:484:LEU:HD11	2.48	0.44
2:B:163:SER:O	2:B:167:ILE:CG2	2.66	0.44
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.98	0.44
2:B:276:VAL:CG1	2:B:276:VAL:O	2.65	0.44
2:B:372:VAL:HA	2:B:389:PHE:CE2	2.53	0.43
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.53	0.43
1:A:168:LEU:O	1:A:172:ARG:HG3	2.17	0.43
2:B:12:LEU:HD11	2:B:127:TYR:CZ	2.53	0.43
2:B:208:HIS:NE2	2:B:212:TRP:CZ3	2.87	0.43
2:B:205:LEU:HD22	2:B:209:LEU:CD1	2.48	0.43
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.53	0.43
1:A:260:LEU:HG	1:A:264:LEU:HD22	2.00	0.43
1:A:406:TRP:CH2	1:A:407:GLN:NE2	2.87	0.43
2:B:66:LYS:CG	2:B:230:MET:HG2	2.45	0.43
1:A:54:ASN:O	1:A:143:ARG:NH2	2.51	0.43
1:A:325:LEU:HD22	1:A:341:ILE:HG22	1.99	0.43
2:B:277:ARG:HG3	2:B:278:GLN:N	2.32	0.43
2:B:173:LYS:C	2:B:176:PRO:HD3	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.74	0.43
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.33	0.43
1:A:5:ILE:CD1	1:A:6:GLU:N	2.81	0.43
2:B:372:VAL:HA	2:B:389:PHE:HE2	1.83	0.43
1:A:210:LEU:HA	1:A:210:LEU:HD12	1.64	0.43
2:B:103:LYS:O	2:B:236:PRO:HG2	2.19	0.43
1:A:465:LYS:HD3	1:A:488:ASP:OD1	2.18	0.43
1:A:193:LEU:HD13	1:A:197:GLN:HG3	2.01	0.43
1:A:38:CYS:O	1:A:47:ILE:HD11	2.19	0.43
2:B:287:LYS:HD3	2:B:291:GLU:OE2	2.19	0.43
1:A:476:LYS:CD	1:A:517:LEU:HD12	2.48	0.43
1:A:345:PRO:C	1:A:347:LYS:H	2.21	0.43
1:A:28:GLU:OE1	1:A:31:ILE:HD12	2.19	0.42
1:A:503:LEU:HD21	1:A:507:GLN:CD	2.39	0.42
1:A:393:ILE:O	1:A:414:TRP:HZ3	2.01	0.42
2:B:188:TYR:CZ	2:B:380:ILE:HG21	2.54	0.42
1:A:125:ARG:NE	1:A:147:ASN:HA	2.34	0.42
2:B:103:LYS:CG	2:B:191:SER:N	2.83	0.42
2:B:350:LYS:HG3	2:B:351:THR:N	2.34	0.42
1:A:311:LYS:O	1:A:313:PRO:HD3	2.20	0.42
2:B:30:LYS:HE2	2:B:404:GLU:OE2	2.19	0.42
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.82	0.42
2:B:24:TRP:HA	2:B:25:PRO:HD3	1.89	0.42
1:A:160:PHE:C	1:A:160:PHE:CD2	2.91	0.42
2:B:257:ILE:O	2:B:260:LEU:HB3	2.20	0.42
1:A:220:LYS:HB3	1:A:220:LYS:NZ	2.34	0.42
1:A:293:ILE:HD12	1:A:293:ILE:N	2.35	0.42
1:A:107:THR:HB	1:A:202:ILE:HD12	2.00	0.42
1:A:433:PRO:HB2	2:B:290:THR:HG23	2.02	0.42
1:A:26:LEU:HB3	1:A:27:THR:H	1.72	0.42
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.35	0.42
2:B:234:LEU:HD21	2:B:377:THR:HG22	2.01	0.42
1:A:470:THR:O	1:A:471:ASP:HB2	2.20	0.42
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.49	0.42
1:A:163:SER:O	1:A:164:MET:C	2.58	0.42
1:A:60:VAL:HG13	1:A:75:VAL:HG22	2.00	0.42
1:A:491:LEU:O	1:A:529:GLU:HB2	2.19	0.42
2:B:207:GLN:HA	2:B:210:LEU:HB2	2.01	0.42
2:B:225:PRO:HA	2:B:226:PRO:HD3	1.31	0.42
2:B:271:TYR:OH	2:B:312:GLU:O	2.30	0.42
1:A:58:THR:HG23	1:A:76:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.78	0.42
1:A:184:MET:HB3	1:A:185:ASP:H	1.66	0.42
2:B:58:THR:HA	2:B:59:PRO:HD3	1.76	0.42
1:A:296:THR:HG22	1:A:297:GLU:H	1.85	0.42
1:A:469:LEU:HD21	1:A:480:GLN:CB	2.49	0.41
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.78	0.41
1:A:54:ASN:OD1	1:A:54:ASN:C	2.56	0.41
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.18	0.41
1:A:434:ILE:HD12	1:A:493:VAL:O	2.20	0.41
2:B:65:LYS:CB	2:B:68:SER:HB3	2.49	0.41
1:A:170:PRO:O	1:A:173:LYS:N	2.50	0.41
2:B:241:VAL:O	2:B:243:PRO:HD3	2.21	0.41
1:A:271:TYR:OH	1:A:313:PRO:HA	2.21	0.41
1:A:494:ASN:HB3	2:B:289:LEU:HD22	2.03	0.41
2:B:282:LEU:HB3	2:B:293:ILE:HG21	2.01	0.41
1:A:399:GLU:O	1:A:403:THR:HB	2.20	0.41
1:A:339:TYR:CE2	1:A:352:GLY:HA3	2.56	0.41
1:A:27:THR:O	1:A:31:ILE:HG13	2.21	0.41
1:A:197:GLN:NE2	1:A:197:GLN:HA	2.35	0.41
2:B:380:ILE:O	2:B:384:GLY:CA	2.69	0.41
1:A:260:LEU:O	1:A:261:VAL:C	2.57	0.41
1:A:90:VAL:O	1:A:91:GLN:O	2.38	0.41
2:B:28:GLU:HA	2:B:135:ILE:HD11	2.02	0.41
1:A:393:ILE:HD12	1:A:423:VAL:CG2	2.50	0.41
1:A:393:ILE:O	1:A:416:PHE:HD1	2.03	0.41
2:B:97:PRO:C	2:B:99:GLY:N	2.74	0.41
2:B:185:ASP:N	2:B:185:ASP:OD2	2.53	0.41
1:A:433:PRO:HB3	2:B:289:LEU:HD23	2.03	0.41
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.43	0.41
1:A:164:MET:O	1:A:168:LEU:CD2	2.69	0.41
1:A:132:ILE:HB	1:A:142:ILE:CG1	2.50	0.41
1:A:5:ILE:CG1	1:A:6:GLU:N	2.84	0.41
1:A:205:LEU:C	1:A:207:GLN:N	2.74	0.41
2:B:193:LEU:N	2:B:193:LEU:HD12	2.36	0.41
1:A:379:SER:C	1:A:381:VAL:N	2.71	0.41
1:A:498:ASP:HA	1:A:536:VAL:O	2.21	0.41
1:A:536:VAL:HA	1:A:537:PRO:HD3	1.90	0.41
1:A:244:ILE:HD13	1:A:244:ILE:O	2.21	0.41
2:B:193:LEU:H	2:B:193:LEU:CD1	2.34	0.41
2:B:157:PRO:O	2:B:161:GLN:N	2.53	0.41
2:B:253:THR:HG23	2:B:256:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PRO:HB3	1:A:235:HIS:NE2	2.36	0.40
1:A:54:ASN:ND2	1:A:129:ALA:HB2	2.36	0.40
1:A:330:GLN:O	1:A:337:TRP:HA	2.21	0.40
2:B:102:LYS:HE3	2:B:102:LYS:HB2	1.85	0.40
2:B:401:TRP:O	2:B:402:TRP:C	2.59	0.40
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.51	0.40
1:A:487:GLN:HA	1:A:524:GLN:NE2	2.36	0.40
2:B:390:LYS:NZ	2:B:415:GLU:OE1	2.53	0.40
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.56	0.40
1:A:362:THR:HG22	1:A:366:LYS:HD3	2.03	0.40
1:A:223:LYS:HB2	1:A:223:LYS:HE3	1.86	0.40
1:A:201:LYS:HA	1:A:204:GLU:HG3	2.03	0.40
1:A:432:GLU:HB2	1:A:433:PRO:HD2	2.02	0.40
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.56	0.40
2:B:205:LEU:HD22	2:B:209:LEU:HG	2.03	0.40
1:A:167:ILE:C	1:A:170:PRO:HD2	2.40	0.40
2:B:168:LEU:C	2:B:168:LEU:HD23	2.41	0.40
2:B:227:PHE:CD2	2:B:231:GLY:CA	3.05	0.40
2:B:193:LEU:HD23	2:B:197:GLN:HB3	2.02	0.40
2:B:375:ILE:HG22	2:B:375:ILE:O	2.21	0.40
2:B:393:ILE:HG12	2:B:394:GLN:N	2.37	0.40
1:A:179:VAL:HG12	4:A:999:NVP:HCB2	2.04	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	506/560 (90%)	447 (88%)	43 (8%)	16 (3%)	5 17
2	B	391/440 (89%)	344 (88%)	44 (11%)	3 (1%)	24 58
All	All	897/1000 (90%)	791 (88%)	87 (10%)	19 (2%)	9 29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	412	PRO
2	B	226	PRO
1	A	90	VAL
1	A	139	THR
1	A	403	THR
1	A	85	GLN
1	A	140	PRO
1	A	141	GLY
1	A	170	PRO
1	A	195	ILE
1	A	243	PRO
1	A	266	TRP
2	B	193	LEU
1	A	52	PRO
1	A	402	TRP
2	B	67	ASP
1	A	321	PRO
1	A	142	ILE

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	462/499 (93%)	409 (88%)	53 (12%)	7	21
2	B	364/400 (91%)	335 (92%)	29 (8%)	15	40
All	All	826/899 (92%)	744 (90%)	82 (10%)	10	28

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	16	MET
1	A	20	LYS

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Mol	Chain	Res	Type
1	A	21	VAL
1	A	52	PRO
1	A	53	GLU
1	A	59	PRO
1	A	61	PHE
1	A	74	LEU
1	A	91	GLN
1	A	105	SER
1	A	109	LEU
1	A	113	ASP
1	A	139	THR
1	A	142	ILE
1	A	160	PHE
1	A	161	GLN
1	A	162	SER
1	A	168	LEU
1	A	177	ASP
1	A	185	ASP
1	A	189	VAL
1	A	194	GLU
1	A	195	ILE
1	A	205	LEU
1	A	244	ILE
1	A	253	THR
1	A	264	LEU
1	A	277	ARG
1	A	287	LYS
1	A	290	THR
1	A	300	GLU
1	A	301	LEU
1	A	317	VAL
1	A	336	GLN
1	A	340	GLN
1	A	356	ARG
1	A	362	THR
1	A	374	LYS
1	A	385	LYS
1	A	394	GLN
1	A	395	LYS
1	A	396	GLU
1	A	402	TRP
1	A	423	VAL

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Mol	Chain	Res	Type
1	A	424	LYS
1	A	470	THR
1	A	473	THR
1	A	476	LYS
1	A	487	GLN
1	A	493	VAL
1	A	517	LEU
2	B	8	VAL
2	B	55	PRO
2	B	60	VAL
2	B	64	LYS
2	B	72	ARG
2	B	123	ASP
2	B	166	LYS
2	B	167	ILE
2	B	168	LEU
2	B	171	PHE
2	B	185	ASP
2	B	201	LYS
2	B	205	LEU
2	B	225	PRO
2	B	227	PHE
2	B	230	MET
2	B	232	TYR
2	B	245	VAL
2	B	249	LYS
2	B	250	ASP
2	B	283	LEU
2	B	286	THR
2	B	289	LEU
2	B	295	LEU
2	B	303	LEU
2	B	353	LYS
2	B	368	LEU
2	B	410	TRP
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	197	GLN

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Mol	Chain	Res	Type
1	A	207	GLN
1	A	222	GLN
1	A	255	ASN
1	A	336	GLN
1	A	373	GLN
1	A	407	GLN
1	A	475	GLN
1	A	480	GLN
1	A	487	GLN
1	A	507	GLN
1	A	509	GLN
1	A	512	GLN
1	A	520	GLN
2	B	57	ASN
2	B	147	ASN
2	B	161	GLN
2	B	235	HIS
2	B	242	GLN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	336	GLN
2	B	348	ASN
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	3,7,8	0.74	0	3,8,10	4.46	1 (33%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	7.49	117.88	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](#)

3 ligands are 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	PO4	A	1300	-	4,4,4	0.91	0	6,6,6	0.27	0
3	PO4	A	1301	-	4,4,4	1.07	0	6,6,6	0.27	0
4	NVP	A	999	-	18,23,23	1.28	4 (22%)	18,34,34	1.10	1 (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	PO4	A	1300	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1301	-	-	0/0/0/0	0/0/0/0
4	NVP	A	999	-	-	0/0/6/6	0/2/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	NVP	C13-N14	2.01	1.36	1.32
4	A	999	NVP	C4-N3	2.11	1.36	1.32
4	A	999	NVP	C12-C11	2.31	1.42	1.36
4	A	999	NVP	C10-C15	2.47	1.43	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	NVP	CC-CA-N1	-2.08	116.11	118.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	PO4	2	0
4	A	999	NVP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	512/560 (91%)	-0.14	16 (3%) 52 40	36, 78, 128, 150	0
2	B	399/440 (90%)	0.09	23 (5%) 26 16	37, 81, 128, 149	0
All	All	911/1000 (91%)	-0.04	39 (4%) 39 27	36, 79, 128, 150	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	468	THR	7.3
1	A	469	LEU	6.9
1	A	470	THR	5.8
1	A	467	VAL	5.0
2	B	67	ASP	4.8
2	B	212	TRP	4.6
1	A	455	ALA	4.3
1	A	138	GLU	4.2
2	B	356	ARG	4.1
1	A	243	PRO	3.9
2	B	190	GLY	3.8
1	A	141	GLY	3.7
1	A	471	ASP	3.6
2	B	211	ARG	3.3
2	B	409	THR	3.1
2	B	240	THR	2.9
2	B	195	ILE	2.9
2	B	197	GLN	2.9
1	A	61	PHE	2.9
1	A	472	THR	2.9
2	B	421	PRO	2.9
2	B	95	PRO	2.8
2	B	225	PRO	2.8
2	B	410	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	428	GLN	2.5
1	A	466	VAL	2.5
2	B	334	GLN	2.4
1	A	242	GLN	2.4
1	A	142	ILE	2.3
1	A	26	LEU	2.3
1	A	402	TRP	2.3
2	B	66	LYS	2.2
2	B	318	TYR	2.2
2	B	317	VAL	2.2
2	B	166	LYS	2.1
2	B	184	MET	2.0
2	B	200	THR	2.0
2	B	167	ILE	2.0
2	B	105	SER	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. 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(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.96	0.14	-	69,76,99,105	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	PO4	A	1300	5/5	0.80	0.30	1.43	149,149,149,149	0
3	PO4	A	1301	5/5	0.75	0.21	1.05	130,140,142,146	0
4	NVP	A	999	20/20	0.97	0.20	0.90	46,59,73,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.