



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:03 PM GMT

PDB ID : 1DTT
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH PETT-2 (PETT130A94)
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Deposited on : 2000-01-13
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

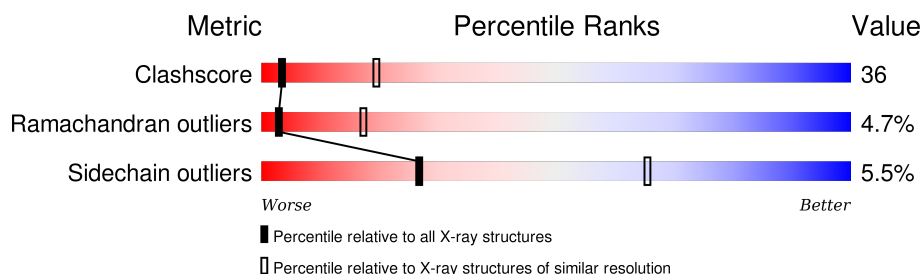
1 Overall quality at a glance

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)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

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
1	CSD	A	280	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7851 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.

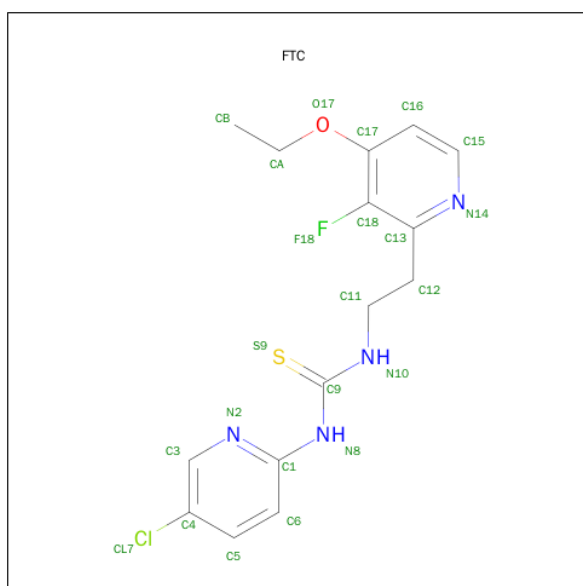
- Molecule 1 is a protein called HIV-1 RT A-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4424	2862	737	817	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3404	2214	565	618	7			

- Molecule 3 is N-[[3-FLUORO-4-ETHOXY-PYRID-2-YL]ETHYL]-N'-[5-CHLORO-PYRIDYL]-THIOUREA (three-letter code: FTC) (formula: C₁₅H₁₆ClFN₄OS).



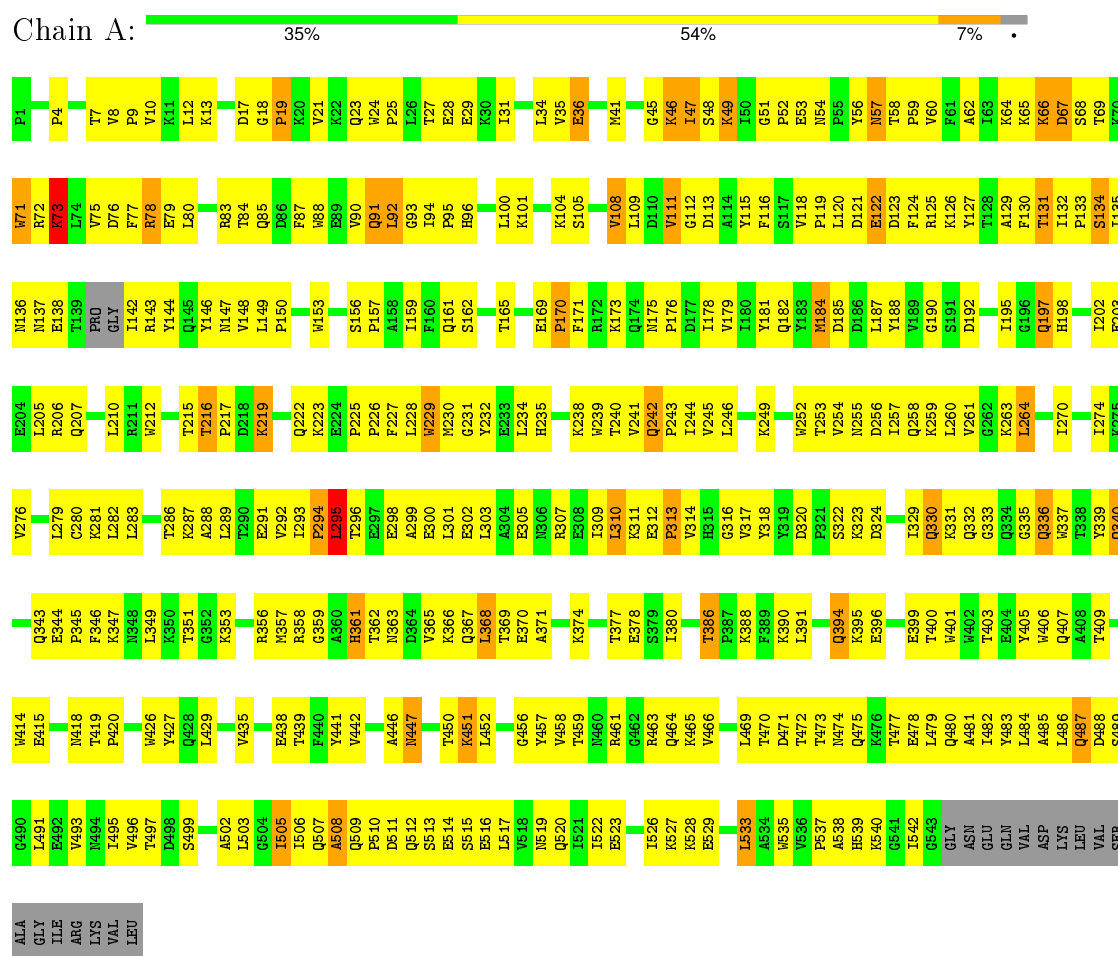
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			23	15	1	1	4	1	1		

3 Residue-property plots

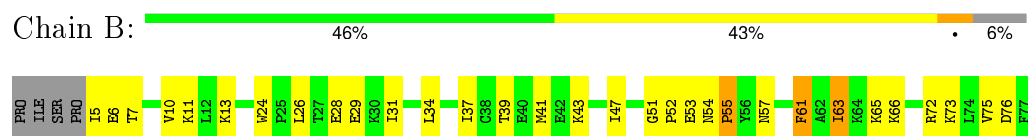
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: HIV-1 RT A-CHAIN



• Molecule 2: HIV-1 RT B-CHAIN





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.70 Å 110.80 Å 73.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	88.5 (30.00-3.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7851	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.40	0/4530	0.65	1/6152 (0.0%)
2	B	0.40	0/3499	0.64	0/4752
All	All	0.40	0/8029	0.65	1/10904 (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	388	LYS	N-CA-C	-5.33	96.62	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	4424	0	4472	376	0
2	B	3404	0	3437	208	0
3	A	23	0	16	2	0
All	All	7851	0	7925	574	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 36.

All (574) 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:216:THR:HG22	1:A:217:PRO:HD2	1.37	1.07
1:A:65:LYS:HD2	1:A:72:ARG:HD3	1.37	1.06
1:A:274:ILE:HD11	1:A:310:LEU:HD11	1.34	1.05
2:B:98:ALA:HA	2:B:101:LYS:HD3	1.37	1.04
1:A:161:GLN:HA	1:A:182:GLN:HE22	1.24	1.00
2:B:358:ARG:HD3	2:B:358:ARG:H	1.29	0.96
1:A:357:MET:HG2	1:A:358:ARG:H	1.30	0.95
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.29	0.95
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.47	0.94
1:A:228:LEU:HD23	1:A:228:LEU:H	1.33	0.94
1:A:23:GLN:HE22	1:A:60:VAL:H	1.14	0.93
2:B:5:ILE:HG22	2:B:6:GLU:H	1.34	0.90
2:B:424:LYS:HD3	2:B:425:LEU:N	1.87	0.88
2:B:98:ALA:CA	2:B:101:LYS:HD3	2.04	0.88
1:A:41:MET:HB3	1:A:46:LYS:HE3	1.57	0.86
2:B:98:ALA:HA	2:B:101:LYS:CD	2.04	0.86
1:A:123:ASP:O	1:A:126:LYS:HD3	1.75	0.86
1:A:489:SER:HB2	1:A:493:VAL:HG21	1.58	0.85
2:B:422:LEU:HD12	2:B:422:LEU:H	1.43	0.83
1:A:65:LYS:HB3	1:A:72:ARG:NH1	1.94	0.83
1:A:245:VAL:HG13	1:A:307:ARG:HD2	1.61	0.82
1:A:361:HIS:CD2	1:A:510:PRO:HB3	2.15	0.81
1:A:57:ASN:HD22	1:A:58:THR:H	1.29	0.81
1:A:57:ASN:HD22	1:A:58:THR:N	1.78	0.81
1:A:356:ARG:HH11	1:A:374:LYS:NZ	1.77	0.81
2:B:88:TRP:HA	2:B:92:LEU:N	1.95	0.80
2:B:169:GLU:O	2:B:173:LYS:HG2	1.81	0.80
1:A:118:VAL:HB	1:A:149:LEU:HD13	1.62	0.80
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.16	0.80
1:A:47:ILE:H	1:A:47:ILE:HD12	1.47	0.80
1:A:441:TYR:HA	1:A:496:VAL:HG22	1.62	0.80
1:A:173:LYS:O	1:A:176:PRO:HD3	1.83	0.79
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.64	0.79
1:A:516:GLU:O	1:A:520:GLN:HG2	1.82	0.79
1:A:75:VAL:HG12	1:A:76:ASP:H	1.48	0.78
1:A:457:TYR:HE2	1:A:465:LYS:HD2	1.49	0.78
1:A:120:LEU:HD12	1:A:121:ASP:H	1.47	0.77
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.67	0.77
1:A:294:PRO:O	1:A:295:LEU:HB2	1.84	0.76
1:A:241:VAL:HG23	1:A:314:VAL:HB	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:CG2	1:A:314:VAL:HB	2.16	0.76
1:A:370:GLU:O	1:A:374:LYS:HG3	1.85	0.75
1:A:260:LEU:HD21	1:A:303:LEU:HD21	1.67	0.75
1:A:366:LYS:O	1:A:369:THR:HB	1.86	0.75
2:B:215:THR:HG22	2:B:217:PRO:HD3	1.69	0.75
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.68	0.75
2:B:119:PRO:HA	2:B:148:VAL:HA	1.67	0.75
1:A:356:ARG:HH11	1:A:374:LYS:HZ1	1.33	0.74
1:A:134:SER:C	1:A:135:ILE:HD12	2.08	0.74
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.23	0.74
2:B:66:LYS:HG3	2:B:407:GLN:NE2	2.03	0.73
1:A:499:SER:HB2	1:A:502:ALA:HB3	1.70	0.73
1:A:122:GLU:H	1:A:122:GLU:CD	1.90	0.73
2:B:242:GLN:HB2	2:B:430:GLU:OE1	1.88	0.73
1:A:75:VAL:HG12	1:A:76:ASP:N	2.03	0.72
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.24	0.72
1:A:282:LEU:O	1:A:293:ILE:HD13	1.89	0.72
1:A:296:THR:O	1:A:299:ALA:HB3	1.88	0.72
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.72	0.72
1:A:132:ILE:HB	1:A:142:ILE:HG22	1.71	0.72
1:A:418:ASN:O	1:A:420:PRO:HD3	1.90	0.72
2:B:353:LYS:NZ	2:B:353:LYS:HB2	2.04	0.71
1:A:125:ARG:HB3	1:A:146:TYR:O	1.89	0.71
1:A:31:ILE:HG13	1:A:134:SER:O	1.90	0.71
1:A:491:LEU:HB3	1:A:529:GLU:HB2	1.70	0.71
2:B:163:SER:O	2:B:167:ILE:HG13	1.91	0.71
2:B:424:LYS:C	2:B:424:LYS:HD3	2.10	0.71
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.24	0.71
1:A:283:LEU:O	1:A:286:THR:HG23	1.91	0.70
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.71	0.70
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.26	0.70
1:A:489:SER:CB	1:A:493:VAL:HG21	2.21	0.70
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.26	0.70
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.74	0.70
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.73	0.70
1:A:48:SER:O	1:A:49:LYS:HB2	1.90	0.69
2:B:380:ILE:O	2:B:384:GLY:N	2.25	0.69
1:A:438:GLU:OE1	1:A:459:THR:HG21	1.91	0.69
2:B:51:GLY:HA3	2:B:53:GLU:OE2	1.92	0.69
2:B:296:THR:HG22	2:B:298:GLU:H	1.57	0.69
1:A:480:GLN:HE22	1:A:483:TYR:HD2	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:HB2	1:A:144:TYR:H	1.58	0.69
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.75	0.69
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.90	0.69
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.20	0.69
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.28	0.68
1:A:293:ILE:CG2	1:A:294:PRO:HD2	2.23	0.68
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.07	0.68
2:B:84:THR:HG21	2:B:153:TRP:NE1	2.06	0.68
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.08	0.68
1:A:76:ASP:OD1	1:A:78:ARG:HG3	1.92	0.68
1:A:485:ALA:O	1:A:489:SER:HB3	1.94	0.68
1:A:506:ILE:H	1:A:506:ILE:HD12	1.57	0.68
1:A:293:ILE:HG23	1:A:294:PRO:HD2	1.75	0.68
2:B:115:TYR:HE1	2:B:157:PRO:HA	1.60	0.67
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.29	0.67
1:A:161:GLN:HA	1:A:182:GLN:NE2	2.05	0.67
1:A:131:THR:HG22	1:A:133:PRO:HD3	1.75	0.67
1:A:295:LEU:HD13	1:A:299:ALA:HB3	1.76	0.67
1:A:116:PHE:O	1:A:148:VAL:HG21	1.95	0.67
1:A:296:THR:HG22	1:A:298:GLU:OE2	1.94	0.67
2:B:11:LYS:O	2:B:85:GLN:HG2	1.94	0.67
1:A:57:ASN:ND2	1:A:58:THR:N	2.42	0.67
1:A:503:LEU:O	1:A:507:GLN:HB2	1.95	0.67
2:B:191:SER:HB2	2:B:193:LEU:HD23	1.77	0.67
1:A:46:LYS:HB2	1:A:147:ASN:HD22	1.59	0.66
2:B:94:ILE:HD12	2:B:95:PRO:HD2	1.77	0.66
2:B:263:LYS:HE2	2:B:425:LEU:HB3	1.78	0.66
1:A:447:ASN:HB3	1:A:450:THR:HG23	1.78	0.66
1:A:451:LYS:HB3	1:A:472:THR:H	1.61	0.66
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.77	0.66
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.77	0.65
1:A:516:GLU:HA	1:A:516:GLU:OE1	1.96	0.65
1:A:243:PRO:HB3	1:A:313:PRO:HG3	1.79	0.65
1:A:27:THR:O	1:A:31:ILE:HG12	1.94	0.65
1:A:274:ILE:CD1	1:A:310:LEU:HD11	2.21	0.65
2:B:209:LEU:HB3	2:B:214:LEU:HD21	1.78	0.65
1:A:295:LEU:HD12	1:A:300:GLU:HG3	1.78	0.65
1:A:210:LEU:CD1	1:A:215:THR:HA	2.26	0.65
1:A:489:SER:HB2	1:A:493:VAL:CG2	2.25	0.65
1:A:111:VAL:HG12	1:A:216:THR:HG23	1.80	0.64
1:A:280:CSD:C	1:A:281:LYS:HA	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.79	0.64
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.32	0.64
1:A:210:LEU:HD13	1:A:215:THR:HA	1.80	0.64
1:A:506:ILE:N	1:A:506:ILE:HD12	2.12	0.64
1:A:396:GLU:O	1:A:400:THR:HG23	1.97	0.63
2:B:358:ARG:HD3	2:B:358:ARG:N	2.08	0.63
2:B:72:ARG:HH21	2:B:151:GLN:NE2	1.97	0.63
1:A:451:LYS:HB3	1:A:472:THR:N	2.13	0.63
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.29	0.63
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.47	0.63
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.80	0.62
1:A:244:ILE:HD13	1:A:263:LYS:HD3	1.82	0.62
1:A:356:ARG:HH22	1:A:371:ALA:HB2	1.64	0.62
2:B:241:VAL:HG22	2:B:242:GLN:N	2.15	0.62
1:A:205:LEU:HD13	1:A:205:LEU:C	2.20	0.62
2:B:194:GLU:HG2	2:B:195:ILE:N	2.14	0.62
1:A:456:GLY:HA3	1:A:466:VAL:HG22	1.81	0.61
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.81	0.61
1:A:287:LYS:HG2	1:A:291:GLU:OE2	2.00	0.61
1:A:65:LYS:HG3	1:A:68:SER:HB2	1.82	0.61
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.35	0.61
1:A:253:THR:O	1:A:256:ASP:HB2	2.00	0.61
1:A:90:VAL:O	1:A:91:GLN:HB2	1.99	0.61
1:A:542:ILE:HD12	1:A:542:ILE:H	1.65	0.60
1:A:506:ILE:CD1	1:A:506:ILE:H	2.14	0.60
1:A:47:ILE:N	1:A:47:ILE:HD12	2.16	0.60
1:A:122:GLU:HA	1:A:125:ARG:HE	1.65	0.60
1:A:47:ILE:H	1:A:47:ILE:CD1	2.14	0.60
2:B:72:ARG:NH2	2:B:151:GLN:HE22	2.00	0.60
1:A:279:LEU:C	1:A:281:LYS:N	2.55	0.60
1:A:64:LYS:HE3	1:A:71:TRP:CE3	2.37	0.60
2:B:422:LEU:HD12	2:B:422:LEU:N	2.16	0.60
1:A:17:ASP:O	1:A:83:ARG:HD3	2.01	0.60
1:A:441:TYR:HA	1:A:496:VAL:CG2	2.32	0.59
1:A:46:LYS:HD2	1:A:46:LYS:O	2.02	0.59
1:A:280:CSD:C	1:A:281:LYS:N	2.66	0.59
2:B:353:LYS:HZ2	2:B:353:LYS:HB2	1.67	0.59
1:A:41:MET:HB3	1:A:46:LYS:CE	2.31	0.59
2:B:213:GLY:C	2:B:214:LEU:HD13	2.23	0.59
1:A:130:PHE:CD1	1:A:144:TYR:HB2	2.38	0.58
2:B:63:ILE:H	2:B:63:ILE:HD13	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:THR:O	1:A:535:TRP:HA	2.03	0.58
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.02	0.58
2:B:233:GLU:O	2:B:234:LEU:HD12	2.03	0.58
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.86	0.58
2:B:120:LEU:HD23	2:B:121:ASP:N	2.19	0.58
1:A:242:GLN:O	1:A:242:GLN:HG2	2.04	0.58
2:B:422:LEU:H	2:B:422:LEU:CD1	2.16	0.58
2:B:168:LEU:O	2:B:172:ARG:HG3	2.03	0.57
1:A:333:GLY:N	1:A:336:GLN:HG3	2.19	0.57
1:A:331:LYS:HG2	1:A:333:GLY:O	2.04	0.57
1:A:65:LYS:HB3	1:A:72:ARG:HH11	1.70	0.57
1:A:184:MET:CE	1:A:184:MET:HA	2.34	0.57
1:A:484:LEU:HD23	1:A:487:GLN:OE1	2.04	0.57
1:A:258:GLN:HE22	1:A:289:LEU:HD11	1.68	0.57
1:A:280:CSD:C	1:A:281:LYS:CA	2.83	0.57
1:A:365:VAL:HG11	1:A:401:TRP:CD2	2.40	0.57
1:A:120:LEU:HD12	1:A:121:ASP:N	2.19	0.57
1:A:64:LYS:HD3	1:A:69:THR:HA	1.85	0.57
1:A:125:ARG:HH11	1:A:147:ASN:HB3	1.67	0.57
1:A:301:LEU:HD23	1:A:301:LEU:O	2.04	0.57
2:B:5:ILE:HG22	2:B:6:GLU:N	2.13	0.56
1:A:295:LEU:CD1	1:A:300:GLU:HG3	2.35	0.56
2:B:210:LEU:HD11	2:B:216:THR:H	1.70	0.56
2:B:65:LYS:NZ	2:B:72:ARG:NH1	2.52	0.56
1:A:92:LEU:C	1:A:92:LEU:HD22	2.26	0.56
1:A:54:ASN:HD22	1:A:126:LYS:HB3	1.70	0.56
2:B:85:GLN:O	2:B:85:GLN:HG3	2.06	0.56
1:A:257:ILE:O	1:A:261:VAL:HG23	2.06	0.56
1:A:75:VAL:CG1	1:A:76:ASP:H	2.18	0.56
1:A:245:VAL:CG1	1:A:307:ARG:HD2	2.33	0.56
2:B:109:LEU:HB2	2:B:187:LEU:HB3	1.88	0.56
2:B:37:ILE:O	2:B:41:MET:HG3	2.05	0.56
1:A:96:HIS:CD2	1:A:230:MET:HE1	2.40	0.56
1:A:517:LEU:O	1:A:520:GLN:HB2	2.06	0.56
1:A:542:ILE:HD12	1:A:542:ILE:N	2.20	0.56
1:A:506:ILE:HG21	1:A:533:LEU:HD12	1.87	0.56
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.05	0.56
2:B:374:LYS:O	2:B:377:THR:HB	2.05	0.56
1:A:56:TYR:O	1:A:129:ALA:HB3	2.05	0.56
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.41	0.56
1:A:249:LYS:HB3	1:A:252:TRP:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:THR:O	2:B:204:GLU:HB2	2.06	0.56
2:B:380:ILE:O	2:B:384:GLY:CA	2.53	0.55
1:A:228:LEU:HG	1:A:228:LEU:O	2.06	0.55
1:A:203:GLU:O	1:A:207:GLN:HG3	2.06	0.55
1:A:340:GLN:HB2	1:A:351:THR:HG22	1.88	0.55
2:B:208:HIS:O	2:B:211:ARG:HB3	2.07	0.55
2:B:109:LEU:HD12	2:B:187:LEU:HD23	1.88	0.55
2:B:356:ARG:HH12	2:B:358:ARG:HA	1.70	0.55
1:A:295:LEU:HD13	1:A:299:ALA:CB	2.37	0.55
2:B:376:THR:O	2:B:380:ILE:HG12	2.06	0.55
1:A:358:ARG:HG2	1:A:512:GLN:HE21	1.72	0.55
1:A:228:LEU:CD2	1:A:228:LEU:H	2.10	0.55
1:A:123:ASP:C	1:A:126:LYS:HD3	2.26	0.55
1:A:64:LYS:HZ3	1:A:69:THR:HG22	1.72	0.55
2:B:233:GLU:C	2:B:234:LEU:HD12	2.26	0.55
1:A:23:GLN:HE22	1:A:60:VAL:N	1.94	0.55
2:B:163:SER:HA	2:B:166:LYS:HE2	1.88	0.55
2:B:65:LYS:HZ2	2:B:72:ARG:HH11	1.53	0.54
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.55	0.54
1:A:66:LYS:HD2	1:A:66:LYS:H	1.72	0.54
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.89	0.54
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.88	0.54
2:B:92:LEU:HD23	2:B:92:LEU:N	2.22	0.54
1:A:514:GLU:HG3	1:A:515:SER:N	2.22	0.54
2:B:97:PRO:O	2:B:98:ALA:HB2	2.08	0.54
2:B:332:GLN:HB2	2:B:336:GLN:HB3	1.90	0.54
1:A:94:ILE:HD12	1:A:94:ILE:N	2.22	0.54
2:B:276:VAL:HG22	2:B:276:VAL:O	2.07	0.54
2:B:96:HIS:ND1	2:B:97:PRO:HD2	2.23	0.54
1:A:23:GLN:NE2	1:A:60:VAL:H	1.94	0.54
1:A:118:VAL:O	1:A:148:VAL:HG23	2.07	0.54
1:A:495:ILE:O	1:A:533:LEU:HD23	2.08	0.53
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.72	0.53
1:A:329:ILE:HG22	1:A:330:GLN:N	2.22	0.53
1:A:57:ASN:N	1:A:143:ARG:HH22	2.05	0.53
2:B:319:TYR:HE1	2:B:321:PRO:HG3	1.68	0.53
1:A:122:GLU:HA	1:A:125:ARG:NE	2.24	0.53
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.72	0.53
1:A:357:MET:HG2	1:A:358:ARG:N	2.12	0.53
1:A:100:LEU:O	1:A:318:TYR:HB3	2.08	0.53
1:A:287:LYS:HG3	1:A:288:ALA:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PRO:CB	1:A:313:PRO:HG3	2.38	0.53
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.43	0.53
1:A:439:THR:O	1:A:459:THR:HA	2.09	0.53
2:B:253:THR:O	2:B:257:ILE:HG12	2.09	0.53
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.09	0.53
2:B:368:LEU:O	2:B:372:VAL:HG23	2.09	0.52
1:A:394:GLN:HG2	1:A:396:GLU:OE2	2.08	0.52
1:A:73:LYS:O	1:A:73:LYS:HD2	2.09	0.52
2:B:61:PHE:CD2	2:B:61:PHE:N	2.78	0.52
2:B:120:LEU:HB2	2:B:148:VAL:O	2.09	0.52
1:A:235:HIS:HB2	1:A:238:LYS:O	2.09	0.52
2:B:425:LEU:O	2:B:429:LEU:HD13	2.10	0.52
1:A:118:VAL:O	1:A:148:VAL:CG2	2.57	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.52
2:B:205:LEU:C	2:B:205:LEU:HD13	2.30	0.52
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.39	0.52
1:A:198:HIS:O	1:A:202:ILE:HG12	2.10	0.52
1:A:149:LEU:H	1:A:149:LEU:HD12	1.75	0.51
1:A:31:ILE:HD12	1:A:133:PRO:O	2.11	0.51
1:A:380:ILE:HD12	1:A:380:ILE:H	1.74	0.51
2:B:332:GLN:OE1	2:B:424:LYS:HE3	2.09	0.51
1:A:54:ASN:ND2	1:A:126:LYS:HB3	2.26	0.51
1:A:340:GLN:HA	1:A:351:THR:HA	1.93	0.51
1:A:523:GLU:HB3	1:A:527:LYS:NZ	2.25	0.51
1:A:77:PHE:O	1:A:78:ARG:C	2.49	0.51
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.92	0.51
1:A:280:CSD:N	1:A:281:LYS:N	2.59	0.51
1:A:27:THR:HG22	1:A:28:GLU:N	2.26	0.51
2:B:333:GLY:O	2:B:336:GLN:HB2	2.11	0.51
1:A:505:ILE:O	1:A:510:PRO:HD3	2.11	0.51
1:A:122:GLU:N	1:A:122:GLU:OE1	2.34	0.51
1:A:197:GLN:HA	1:A:197:GLN:HE21	1.75	0.51
2:B:121:ASP:OD1	2:B:122:GLU:N	2.44	0.51
2:B:205:LEU:O	2:B:205:LEU:HD13	2.11	0.51
1:A:463:ARG:C	1:A:464:GLN:HG3	2.31	0.51
2:B:99:GLY:O	2:B:102:LYS:N	2.44	0.51
1:A:260:LEU:O	1:A:264:LEU:HD23	2.11	0.51
1:A:243:PRO:HG3	1:A:313:PRO:HG3	1.93	0.50
1:A:170:PRO:HG2	1:A:171:PHE:H	1.75	0.50
1:A:17:ASP:OD2	1:A:18:GLY:N	2.43	0.50
1:A:357:MET:CG	1:A:358:ARG:H	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ALA:HB1	1:A:71:TRP:CD1	2.45	0.50
2:B:332:GLN:NE2	2:B:424:LYS:HG2	2.27	0.50
1:A:480:GLN:HE21	1:A:484:LEU:HG	1.76	0.50
1:A:244:ILE:CD1	1:A:263:LYS:HD3	2.41	0.50
2:B:267:ALA:CB	2:B:426:TRP:CH2	2.95	0.50
2:B:214:LEU:O	2:B:215:THR:C	2.50	0.50
2:B:406:TRP:O	2:B:407:GLN:HG3	2.12	0.50
2:B:380:ILE:O	2:B:384:GLY:HA2	2.10	0.50
1:A:46:LYS:O	1:A:48:SER:N	2.44	0.50
2:B:115:TYR:CE1	2:B:157:PRO:HA	2.43	0.50
1:A:130:PHE:O	1:A:143:ARG:HG3	2.12	0.50
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.93	0.50
1:A:441:TYR:CD2	1:A:496:VAL:HG21	2.47	0.49
2:B:168:LEU:C	2:B:172:ARG:HG3	2.33	0.49
1:A:243:PRO:CG	1:A:313:PRO:HG3	2.42	0.49
1:A:480:GLN:O	1:A:483:TYR:HB3	2.12	0.49
1:A:109:LEU:N	1:A:109:LEU:HD12	2.27	0.49
1:A:513:SER:HB3	1:A:519:ASN:ND2	2.26	0.49
1:A:310:LEU:N	1:A:310:LEU:HD12	2.28	0.49
2:B:244:ILE:HG13	2:B:426:TRP:HZ2	1.75	0.49
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.94	0.49
1:A:179:VAL:HG11	3:A:999:FTC:H112	1.93	0.49
2:B:39:THR:O	2:B:43:LYS:HG2	2.12	0.49
1:A:537:PRO:CG	2:B:262:GLY:HA2	2.43	0.49
2:B:244:ILE:HG21	2:B:426:TRP:CZ2	2.48	0.49
1:A:474:ASN:OD1	1:A:475:GLN:HG3	2.13	0.49
2:B:101:LYS:HG2	2:B:382:ILE:HA	1.95	0.49
2:B:98:ALA:C	2:B:101:LYS:HD3	2.34	0.48
2:B:424:LYS:HD3	2:B:425:LEU:CA	2.42	0.48
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.94	0.48
1:A:197:GLN:NE2	1:A:197:GLN:HA	2.28	0.48
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.94	0.48
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.42	0.48
2:B:191:SER:OG	2:B:198:HIS:ND1	2.40	0.48
1:A:13:LYS:HE3	1:A:84:THR:O	2.13	0.48
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.46	0.48
2:B:393:ILE:O	2:B:416:PHE:HB3	2.13	0.48
1:A:474:ASN:O	1:A:478:GLU:HG3	2.13	0.48
1:A:367:GLN:O	1:A:368:LEU:C	2.52	0.48
1:A:324:ASP:O	1:A:343:GLN:HG2	2.14	0.48
1:A:442:VAL:HG22	1:A:496:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:O	1:A:243:PRO:HD3	2.14	0.48
2:B:65:LYS:HZ2	2:B:72:ARG:NH1	2.10	0.48
1:A:320:ASP:OD1	1:A:323:LYS:HG2	2.14	0.48
1:A:427:TYR:CE2	1:A:509:GLN:HG3	2.49	0.48
1:A:245:VAL:HG13	1:A:307:ARG:CD	2.38	0.48
1:A:235:HIS:HB2	1:A:238:LYS:HG2	1.96	0.48
1:A:229:TRP:HA	1:A:229:TRP:CE3	2.47	0.48
2:B:10:VAL:HG12	2:B:11:LYS:N	2.29	0.48
2:B:28:GLU:O	2:B:31:ILE:N	2.46	0.48
1:A:312:GLU:HG3	1:A:312:GLU:O	2.13	0.48
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.49	0.48
1:A:457:TYR:CE2	1:A:465:LYS:HD2	2.38	0.48
1:A:470:THR:O	1:A:471:ASP:HB3	2.13	0.48
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.49	0.48
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.96	0.47
1:A:87:PHE:N	1:A:87:PHE:CD1	2.82	0.47
1:A:356:ARG:NH1	1:A:374:LYS:NZ	2.55	0.47
2:B:175:ASN:C	2:B:177:ASP:H	2.17	0.47
2:B:279:LEU:HG	2:B:302:GLU:OE2	2.14	0.47
1:A:311:LYS:O	1:A:313:PRO:HD3	2.14	0.47
1:A:36:GLU:O	1:A:36:GLU:HG2	2.13	0.47
1:A:472:THR:OG1	1:A:473:THR:N	2.47	0.47
1:A:181:TYR:HB3	1:A:188:TYR:HB2	1.97	0.47
2:B:399:GLU:HA	2:B:402:TRP:HD1	1.79	0.47
1:A:474:ASN:CG	1:A:475:GLN:N	2.67	0.47
2:B:296:THR:HG22	2:B:298:GLU:N	2.26	0.47
1:A:66:LYS:N	1:A:66:LYS:HD2	2.30	0.47
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.29	0.47
1:A:345:PRO:O	1:A:346:PHE:HB2	2.15	0.47
1:A:130:PHE:O	1:A:143:ARG:NH1	2.48	0.47
1:A:520:GLN:HA	1:A:520:GLN:OE1	2.14	0.47
1:A:282:LEU:H	1:A:282:LEU:HD22	1.79	0.47
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.13	0.47
1:A:4:PRO:HG2	1:A:212:TRP:CZ3	2.49	0.47
2:B:318:TYR:HE1	2:B:320:ASP:HB2	1.80	0.47
1:A:255:ASN:O	1:A:259:LYS:HG3	2.15	0.47
1:A:491:LEU:O	1:A:529:GLU:HB3	2.15	0.47
1:A:452:LEU:HD12	1:A:469:LEU:O	2.14	0.47
2:B:231:GLY:O	2:B:232:TYR:HB2	2.15	0.47
1:A:506:ILE:CD1	1:A:506:ILE:N	2.77	0.47
1:A:240:THR:HA	1:A:314:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:O	1:A:138:GLU:HB3	2.15	0.47
1:A:8:VAL:HG21	1:A:159:ILE:HG12	1.97	0.47
2:B:254:VAL:O	2:B:258:GLN:HG3	2.15	0.47
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.44	0.47
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.15	0.47
1:A:51:GLY:O	1:A:53:GLU:N	2.48	0.47
1:A:149:LEU:H	1:A:149:LEU:CD1	2.28	0.46
1:A:149:LEU:HD12	1:A:149:LEU:N	2.30	0.46
1:A:507:GLN:C	1:A:509:GLN:H	2.18	0.46
1:A:451:LYS:O	1:A:471:ASP:N	2.45	0.46
1:A:340:GLN:CB	1:A:351:THR:HG22	2.44	0.46
2:B:63:ILE:HD13	2:B:63:ILE:N	2.30	0.46
1:A:361:HIS:ND1	1:A:361:HIS:C	2.69	0.46
2:B:120:LEU:HD21	2:B:124:PHE:HB3	1.97	0.46
1:A:477:THR:O	1:A:480:GLN:HB3	2.15	0.46
2:B:376:THR:CG2	2:B:386:THR:HG22	2.45	0.46
1:A:450:THR:O	1:A:452:LEU:N	2.48	0.46
2:B:7:THR:O	2:B:7:THR:HG23	2.15	0.46
1:A:101:LYS:O	3:A:999:FTC:H6	2.16	0.46
1:A:505:ILE:O	1:A:510:PRO:CD	2.64	0.46
1:A:226:PRO:HA	1:A:234:LEU:O	2.15	0.46
2:B:125:ARG:NE	2:B:147:ASN:HA	2.31	0.46
1:A:317:VAL:O	1:A:349:LEU:HD23	2.15	0.46
2:B:317:VAL:O	2:B:317:VAL:HG23	2.16	0.46
1:A:339:TYR:CD1	1:A:339:TYR:C	2.89	0.46
2:B:155:GLY:O	2:B:158:ALA:HB3	2.15	0.46
2:B:52:PRO:HD2	2:B:53:GLU:OE2	2.16	0.46
2:B:63:ILE:O	2:B:72:ARG:HB3	2.16	0.46
1:A:507:GLN:O	1:A:509:GLN:N	2.43	0.46
1:A:92:LEU:HD21	2:B:137:ASN:OD1	2.16	0.46
1:A:337:TRP:O	1:A:353:LYS:HA	2.15	0.46
1:A:171:PHE:CD1	1:A:205:LEU:HD23	2.51	0.46
1:A:241:VAL:HG11	1:A:270:ILE:HD13	1.98	0.46
2:B:121:ASP:C	2:B:121:ASP:OD1	2.55	0.46
1:A:31:ILE:HG21	1:A:134:SER:HA	1.97	0.46
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.99	0.46
2:B:171:PHE:CG	2:B:205:LEU:HD23	2.51	0.46
1:A:320:ASP:OD2	1:A:322:SER:HB3	2.15	0.46
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.50	0.45
2:B:165:THR:OG1	2:B:166:LYS:N	2.49	0.45
2:B:194:GLU:HG2	2:B:196:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD12	1:A:83:ARG:O	2.16	0.45
1:A:118:VAL:HB	1:A:149:LEU:CD1	2.40	0.45
1:A:92:LEU:HD13	1:A:93:GLY:N	2.31	0.45
1:A:64:LYS:NZ	1:A:69:THR:HG22	2.30	0.45
1:A:301:LEU:O	1:A:305:GLU:HB2	2.16	0.45
2:B:78:ARG:HD3	2:B:411:ILE:O	2.17	0.45
1:A:120:LEU:CD1	1:A:121:ASP:H	2.24	0.45
2:B:121:ASP:OD1	2:B:123:ASP:N	2.48	0.45
1:A:162:SER:O	1:A:165:THR:HB	2.16	0.45
1:A:77:PHE:O	1:A:80:LEU:N	2.49	0.45
2:B:158:ALA:O	2:B:161:GLN:HB2	2.16	0.45
2:B:206:ARG:HG3	2:B:216:THR:O	2.17	0.45
2:B:26:LEU:HD12	2:B:133:PRO:HG3	1.98	0.45
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.98	0.45
1:A:46:LYS:HD2	1:A:48:SER:HB3	1.98	0.45
1:A:399:GLU:O	1:A:403:THR:HG23	2.17	0.45
2:B:383:TRP:O	2:B:384:GLY:C	2.54	0.45
1:A:361:HIS:NE2	1:A:508:ALA:HB1	2.32	0.45
1:A:474:ASN:O	1:A:477:THR:OG1	2.27	0.45
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.45	0.45
2:B:255:ASN:O	2:B:259:LYS:HG3	2.17	0.45
1:A:124:PHE:O	1:A:125:ARG:C	2.54	0.45
1:A:7:THR:HG22	1:A:119:PRO:O	2.17	0.45
2:B:393:ILE:HG12	2:B:394:GLN:N	2.32	0.45
1:A:419:THR:HG23	1:A:419:THR:O	2.17	0.45
1:A:505:ILE:HG22	1:A:506:ILE:HD12	1.99	0.45
1:A:171:PHE:CG	1:A:205:LEU:HD23	2.52	0.45
1:A:129:ALA:HB1	1:A:143:ARG:CZ	2.47	0.44
2:B:79:GLU:O	2:B:83:ARG:HG3	2.17	0.44
1:A:49:LYS:HA	1:A:144:TYR:HA	1.98	0.44
1:A:309:ILE:C	1:A:311:LYS:H	2.21	0.44
2:B:241:VAL:HG22	2:B:242:GLN:H	1.81	0.44
1:A:514:GLU:HG3	1:A:515:SER:H	1.82	0.44
1:A:317:VAL:HG22	1:A:318:TYR:N	2.32	0.44
2:B:116:PHE:O	2:B:117:SER:C	2.54	0.44
1:A:229:TRP:O	1:A:231:GLY:N	2.48	0.44
2:B:100:LEU:HA	2:B:103:LYS:HB2	2.00	0.44
2:B:426:TRP:O	2:B:429:LEU:HB2	2.17	0.44
1:A:47:ILE:HG22	1:A:47:ILE:O	2.16	0.44
2:B:209:LEU:C	2:B:211:ARG:N	2.70	0.44
1:A:329:ILE:HD12	1:A:391:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:GLN:C	2:B:336:GLN:H	2.21	0.44
2:B:193:LEU:HD22	2:B:193:LEU:N	2.33	0.44
1:A:542:ILE:H	1:A:542:ILE:CD1	2.31	0.44
1:A:126:LYS:H	1:A:126:LYS:HG3	1.57	0.44
2:B:203:GLU:O	2:B:207:GLN:HG3	2.17	0.44
2:B:126:LYS:HG3	2:B:127:TYR:N	2.32	0.44
1:A:254:VAL:CG2	1:A:291:GLU:HB3	2.48	0.44
1:A:171:PHE:CE1	1:A:205:LEU:HB2	2.51	0.44
2:B:374:LYS:O	2:B:378:GLU:HG3	2.17	0.44
1:A:216:THR:HG22	1:A:217:PRO:CD	2.26	0.44
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.99	0.44
1:A:95:PRO:HG3	2:B:137:ASN:O	2.17	0.44
1:A:344:GLU:HB2	1:A:347:LYS:HB2	2.00	0.44
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.53	0.43
1:A:451:LYS:HD2	1:A:472:THR:O	2.17	0.43
1:A:451:LYS:CB	1:A:471:ASP:HA	2.48	0.43
1:A:169:GLU:N	1:A:170:PRO:HD2	2.33	0.43
2:B:52:PRO:C	2:B:54:ASN:N	2.69	0.43
1:A:64:LYS:HG3	1:A:71:TRP:CE2	2.53	0.43
1:A:230:MET:O	1:A:232:TYR:CD1	2.72	0.43
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.99	0.43
1:A:458:VAL:HA	1:A:463:ARG:O	2.18	0.43
2:B:268:SER:HA	2:B:271:TYR:O	2.18	0.43
1:A:46:LYS:NZ	1:A:48:SER:OG	2.50	0.43
2:B:206:ARG:O	2:B:210:LEU:HD13	2.18	0.43
2:B:115:TYR:HE2	2:B:185:ASP:HA	1.82	0.43
2:B:13:LYS:HE2	2:B:86:ASP:OD2	2.19	0.43
1:A:282:LEU:N	1:A:282:LEU:HD22	2.34	0.43
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.80	0.43
1:A:435:VAL:HA	2:B:290:THR:HG21	2.00	0.43
1:A:66:LYS:O	1:A:67:ASP:HB2	2.19	0.43
1:A:270:ILE:HG22	1:A:314:VAL:HG21	2.01	0.43
1:A:409:THR:O	2:B:364:ASP:HB2	2.18	0.43
1:A:184:MET:HB3	1:A:185:ASP:H	1.50	0.43
2:B:87:PHE:CD1	2:B:87:PHE:N	2.87	0.43
2:B:75:VAL:HG12	2:B:76:ASP:N	2.33	0.43
2:B:214:LEU:HD13	2:B:214:LEU:N	2.34	0.43
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.81	0.43
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.49	0.42
1:A:23:GLN:NE2	1:A:59:PRO:HA	2.34	0.42
1:A:359:GLY:C	1:A:361:HIS:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:O	2:B:195:ILE:HG12	2.19	0.42
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.91	0.42
1:A:19:PRO:HG3	1:A:83:ARG:HD2	2.00	0.42
1:A:175:ASN:HB3	1:A:178:ILE:HD12	2.01	0.42
1:A:7:THR:HG21	1:A:120:LEU:O	2.19	0.42
2:B:245:VAL:HG13	2:B:245:VAL:O	2.19	0.42
1:A:111:VAL:O	1:A:111:VAL:HG23	2.18	0.42
2:B:173:LYS:O	2:B:176:PRO:HD3	2.20	0.42
1:A:303:LEU:HA	1:A:303:LEU:HD23	1.91	0.42
1:A:366:LYS:HD3	1:A:405:TYR:OH	2.19	0.42
1:A:27:THR:HG22	1:A:28:GLU:H	1.85	0.42
2:B:241:VAL:CG2	2:B:242:GLN:N	2.81	0.42
1:A:115:TYR:O	1:A:149:LEU:HB2	2.19	0.42
1:A:258:GLN:HE22	1:A:289:LEU:CD1	2.33	0.42
2:B:345:PRO:O	2:B:346:PHE:HB2	2.20	0.42
2:B:358:ARG:CD	2:B:358:ARG:H	2.10	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
1:A:480:GLN:NE2	1:A:483:TYR:HD2	2.11	0.42
1:A:219:LYS:HA	1:A:222:GLN:CD	2.40	0.42
2:B:180:ILE:HA	2:B:188:TYR:O	2.19	0.42
1:A:452:LEU:HA	1:A:469:LEU:O	2.20	0.42
2:B:209:LEU:O	2:B:210:LEU:C	2.58	0.42
1:A:478:GLU:HB3	1:A:499:SER:OG	2.20	0.42
2:B:201:LYS:HE2	2:B:204:GLU:OE2	2.19	0.42
1:A:426:TRP:O	1:A:427:TYR:HB3	2.20	0.42
1:A:92:LEU:O	1:A:92:LEU:HD22	2.20	0.42
2:B:326:ILE:CG2	2:B:327:ALA:N	2.82	0.42
2:B:164:MET:HE3	2:B:168:LEU:HG	2.00	0.42
1:A:309:ILE:O	1:A:311:LYS:N	2.53	0.42
1:A:345:PRO:C	1:A:346:PHE:HD1	2.23	0.42
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.42
1:A:390:LYS:HE2	1:A:415:GLU:OE2	2.20	0.42
1:A:486:LEU:HA	1:A:528:LYS:HE3	2.02	0.42
1:A:489:SER:OG	1:A:493:VAL:HG21	2.19	0.41
1:A:12:LEU:O	1:A:13:LYS:C	2.57	0.41
1:A:225:PRO:HA	1:A:226:PRO:C	2.41	0.41
1:A:206:ARG:HG2	1:A:206:ARG:NH1	2.35	0.41
2:B:97:PRO:HG2	2:B:100:LEU:CD2	2.50	0.41
1:A:241:VAL:O	1:A:243:PRO:CD	2.69	0.41
2:B:161:GLN:O	2:B:164:MET:HB3	2.20	0.41
2:B:175:ASN:CG	2:B:201:LYS:HZ1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PRO:HG3	2:B:262:GLY:HA2	2.03	0.41
2:B:79:GLU:O	2:B:82:LYS:HB2	2.20	0.41
1:A:129:ALA:CB	1:A:143:ARG:NH2	2.83	0.41
1:A:253:THR:HG22	1:A:292:VAL:HG22	2.03	0.41
2:B:120:LEU:HD12	2:B:150:PRO:HD3	2.01	0.41
2:B:371:ALA:O	2:B:372:VAL:C	2.59	0.41
2:B:34:LEU:HD21	2:B:73:LYS:HG3	2.02	0.41
1:A:105:SER:O	1:A:190:GLY:HA2	2.21	0.41
2:B:380:ILE:HA	2:B:384:GLY:HA2	2.01	0.41
1:A:479:LEU:O	1:A:482:ILE:HB	2.20	0.41
1:A:522:ILE:O	1:A:526:ILE:HG13	2.20	0.41
2:B:100:LEU:HD23	2:B:100:LEU:N	2.36	0.41
1:A:358:ARG:CD	1:A:512:GLN:HE21	2.33	0.41
2:B:168:LEU:O	2:B:169:GLU:C	2.59	0.41
1:A:451:LYS:O	1:A:471:ASP:HA	2.21	0.41
2:B:206:ARG:HG2	2:B:206:ARG:NH1	2.36	0.41
2:B:65:LYS:HZ1	2:B:72:ARG:HH12	1.67	0.41
2:B:193:LEU:H	2:B:193:LEU:HD22	1.86	0.41
1:A:363:ASN:OD1	1:A:365:VAL:HB	2.20	0.41
2:B:28:GLU:O	2:B:29:GLU:C	2.57	0.41
1:A:104:LYS:HB2	1:A:192:ASP:HA	2.02	0.41
2:B:252:TRP:HB3	2:B:257:ILE:HD11	2.02	0.41
1:A:358:ARG:CZ	1:A:358:ARG:HB2	2.51	0.40
2:B:267:ALA:C	2:B:269:GLN:H	2.24	0.40
1:A:291:GLU:HG2	1:A:292:VAL:N	2.36	0.40
1:A:27:THR:HG22	1:A:29:GLU:H	1.86	0.40
1:A:361:HIS:HE2	1:A:508:ALA:HB1	1.85	0.40
1:A:505:ILE:HG22	1:A:506:ILE:N	2.36	0.40
2:B:360:ALA:CB	2:B:366:LYS:HD3	2.43	0.40
1:A:35:VAL:HG12	1:A:36:GLU:N	2.35	0.40
1:A:18:GLY:HA2	1:A:19:PRO:HD3	1.97	0.40
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.21	0.40
2:B:53:GLU:O	2:B:55:PRO:HD3	2.21	0.40
1:A:91:GLN:C	1:A:93:GLY:N	2.74	0.40
1:A:46:LYS:CB	1:A:147:ASN:HD22	2.33	0.40
1:A:118:VAL:CG1	1:A:119:PRO:HD2	2.50	0.40
1:A:254:VAL:HG22	1:A:293:ILE:HD11	2.03	0.40
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.51	0.40
2:B:98:ALA:O	2:B:101:LYS:HD3	2.21	0.40
1:A:77:PHE:O	1:A:79:GLU:N	2.55	0.40
2:B:78:ARG:O	2:B:82:LYS:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:THR:O	1:A:378:GLU:C	2.59	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	535/560 (96%)	422 (79%)	79 (15%)	34 (6%)	2	9
2	B	406/440 (92%)	338 (83%)	58 (14%)	10 (2%)	7	34
All	All	941/1000 (94%)	760 (81%)	137 (15%)	44 (5%)	3	17

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	PRO
1	A	47	ILE
1	A	49	LYS
1	A	67	ASP
1	A	73	LYS
1	A	134	SER
1	A	294	PRO
1	A	295	LEU
1	A	451	LYS
1	A	487	GLN
1	A	505	ILE
1	A	538	ALA
2	B	97	PRO
2	B	98	ALA
2	B	232	TYR
1	A	52	PRO
1	A	66	LYS

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Mol	Chain	Res	Type
1	A	85	GLN
1	A	112	GLY
1	A	195	ILE
1	A	310	LEU
1	A	313	PRO
1	A	508	ALA
1	A	540	LYS
2	B	215	THR
2	B	358	ARG
1	A	45	GLY
1	A	78	ARG
1	A	131	THR
1	A	136	ASN
1	A	539	HIS
2	B	214	LEU
2	B	241	VAL
2	B	356	ARG
1	A	91	GLN
1	A	113	ASP
1	A	127	TYR
1	A	242	GLN
1	A	276	VAL
1	A	111	VAL
2	B	431	LYS
1	A	25	PRO
1	A	170	PRO
2	B	176	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	484/499 (97%)	454 (94%)	30 (6%)	23	60
2	B	374/400 (94%)	357 (96%)	17 (4%)	34	74
All	All	858/899 (95%)	811 (94%)	47 (6%)	27	65

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	36	GLU
1	A	46	LYS
1	A	57	ASN
1	A	71	TRP
1	A	73	LYS
1	A	88	TRP
1	A	92	LEU
1	A	108	VAL
1	A	122	GLU
1	A	150	PRO
1	A	184	MET
1	A	197	GLN
1	A	216	THR
1	A	219	LYS
1	A	229	TRP
1	A	264	LEU
1	A	295	LEU
1	A	330	GLN
1	A	332	GLN
1	A	336	GLN
1	A	340	GLN
1	A	361	HIS
1	A	362	THR
1	A	368	LEU
1	A	386	THR
1	A	394	GLN
1	A	447	ASN
1	A	488	ASP
1	A	533	LEU
2	B	24	TRP
2	B	55	PRO
2	B	61	PHE
2	B	63	ILE
2	B	88	TRP
2	B	92	LEU
2	B	139	THR
2	B	161	GLN
2	B	184	MET
2	B	214	LEU
2	B	283	LEU
2	B	336	GLN

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Mol	Chain	Res	Type
2	B	358	ARG
2	B	368	LEU
2	B	422	LEU
2	B	424	LYS
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	137	ASN
1	A	145	GLN
1	A	147	ASN
1	A	174	GLN
1	A	182	GLN
1	A	197	GLN
1	A	207	GLN
1	A	255	ASN
1	A	258	GLN
1	A	332	GLN
1	A	340	GLN
1	A	394	GLN
1	A	428	GLN
1	A	447	ASN
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
1	A	512	GLN
1	A	519	ASN
2	B	57	ASN
2	B	147	ASN
2	B	151	GLN
2	B	174	GLN
2	B	255	ASN
2	B	269	GLN
2	B	278	GLN
2	B	348	ASN
2	B	407	GLN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	A	280	1	3,7,8	0.63	0	3,8,10	2.97	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	4.81	113.41	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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	4	0

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	FTC	A	999	-	23,24,24	1.69	6 (26%)	29,31,31	2.23	12 (41%)

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	FTC	A	999	-	-	0/13/13/13	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FTC	C1-N8	-2.19	1.36	1.40
3	A	999	FTC	C3-N2	2.44	1.39	1.34
3	A	999	FTC	C18-C13	2.61	1.41	1.38
3	A	999	FTC	C9-S9	2.70	1.74	1.68
3	A	999	FTC	C1-N2	3.11	1.40	1.34
3	A	999	FTC	C13-N14	3.94	1.38	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	999	FTC	C16-C15-N14	-4.18	119.13	123.90
3	A	999	FTC	C4-C3-N2	-3.84	117.55	122.32
3	A	999	FTC	O17-C17-C16	-2.95	117.85	124.01
3	A	999	FTC	CA-O17-C17	-2.69	112.99	118.01
3	A	999	FTC	C6-C1-N8	-2.58	115.85	123.04
3	A	999	FTC	C6-C1-N2	-2.10	119.07	122.49
3	A	999	FTC	F18-C18-C13	2.19	121.00	118.11
3	A	999	FTC	C6-C5-C4	2.45	121.95	119.23
3	A	999	FTC	O17-C17-C18	2.73	121.49	115.97
3	A	999	FTC	N8-C1-N2	3.50	124.92	114.83
3	A	999	FTC	C15-N14-C13	3.74	123.17	117.73
3	A	999	FTC	C3-N2-C1	4.54	122.85	117.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	FTC	2	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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.