



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:56 am GMT

PDB ID : 1RTJ  
Title : MECHANISM OF INHIBITION OF HIV-1 REVERSE TRANSCRIPTASE  
BY NON-NUCLEOSIDE INHIBITORS  
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Deposited on : 1995-05-03  
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

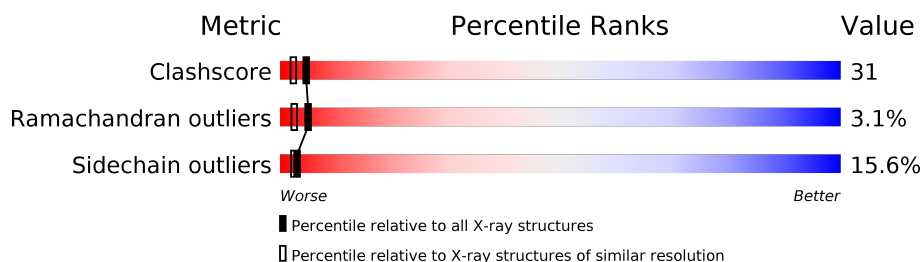
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

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

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8210 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	543	Total	C	N	O	S	0	0	0
			4435	2869	739	819	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	0	0
			3508	2282	580	639	7			

- Molecule 3 is water.

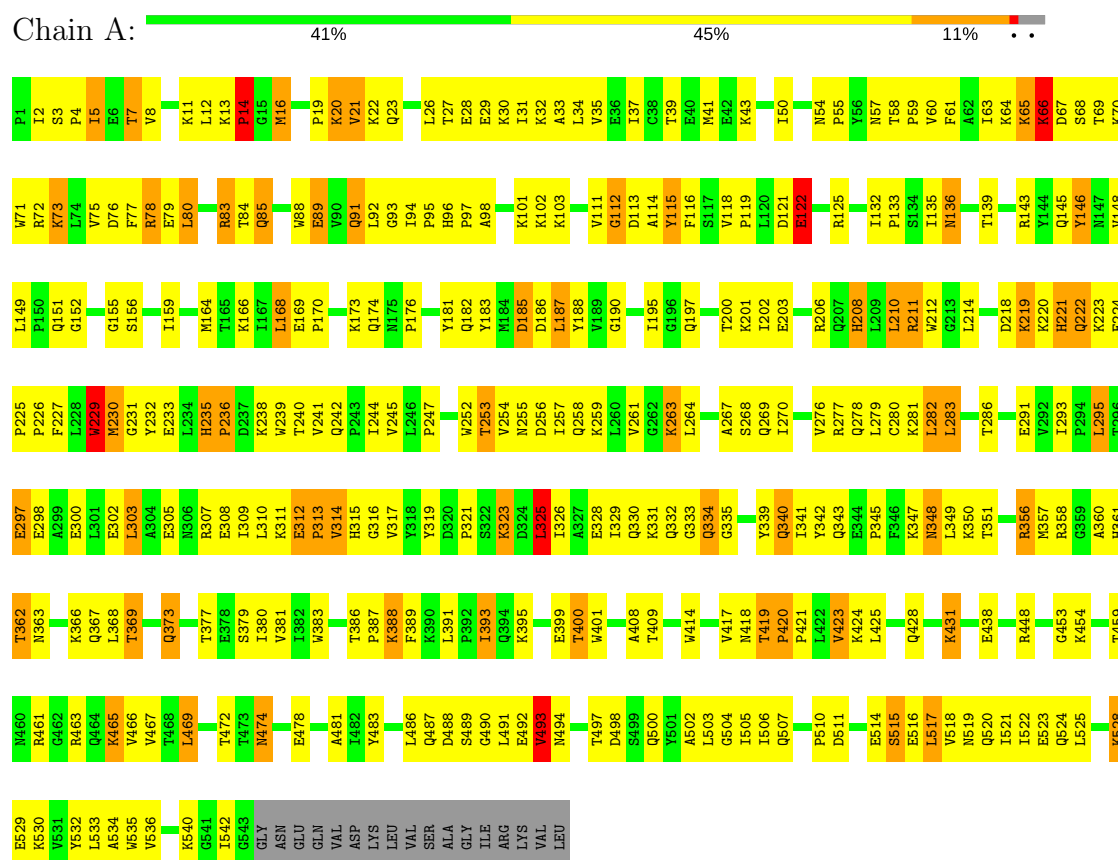
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		
3	B	103	Total	O	0	0
			103	103		

### 3 Residue-property plots

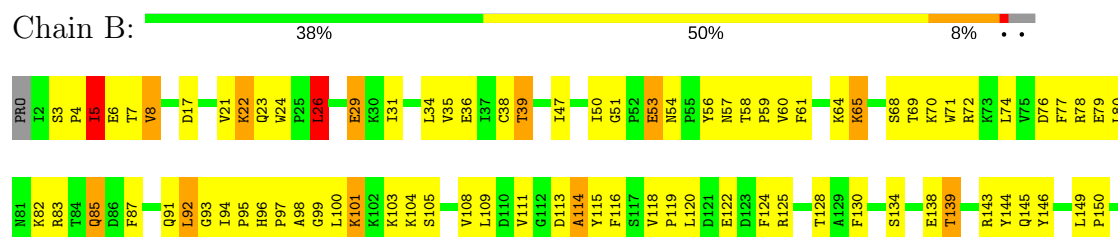
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE



#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.50Å 109.40Å 72.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.35	Depositor
% Data completeness (in resolution range)	89.5 (25.00-2.35)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.219 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	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

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	0.75	0/4544	0.94	7/6175 (0.1%)
2	B	0.75	0/3607	0.92	3/4903 (0.1%)
All	All	0.75	0/8151	0.94	10/11078 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	1
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	LEU	CA-CB-CG	-7.04	99.12	115.30
1	A	139	THR	N-CA-C	-5.91	95.05	111.00
1	A	494	ASN	N-CA-C	-5.76	95.45	111.00
1	A	388	LYS	N-CA-C	-5.72	95.56	111.00
2	B	93	GLY	N-CA-C	-5.52	99.31	113.10
1	A	333	GLY	N-CA-C	-5.41	99.58	113.10
2	B	26	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	493	VAL	CB-CA-C	-5.21	101.50	111.40
2	B	214	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	325	LEU	N-CA-C	-5.10	97.22	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	TYR	Sidechain
1	A	146	TYR	Sidechain
1	A	319	TYR	Sidechain
2	B	56	TYR	Sidechain

## 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	4435	0	4483	277	0
2	B	3508	0	3541	225	0
3	A	164	0	0	7	0
3	B	103	0	0	5	0
All	All	8210	0	8024	495	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 (495) 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)
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.40	1.00
1:A:342:TYR:HB3	1:A:348:ASN:HB3	1.47	0.97
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.47	0.96
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.52	0.92
1:A:14:PRO:HG2	3:A:1024:HOH:O	1.73	0.89
2:B:303:LEU:HD13	2:B:307:ARG:HH21	1.38	0.89
1:A:335:GLY:O	1:A:356:ARG:HB2	1.73	0.88
1:A:515:SER:OG	1:A:518:VAL:HG23	1.73	0.88
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.55	0.88
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.57	0.86
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.11	0.86
1:A:502:ALA:O	1:A:506:ILE:HG13	1.76	0.84
1:A:112:GLY:HA2	1:A:185:ASP:HB3	1.59	0.82
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:HIS:CE1	1:A:212:TRP:HE1	1.98	0.82
1:A:542:ILE:HG13	2:B:283:LEU:HD23	1.60	0.81
1:A:229:TRP:HB3	1:A:232:TYR:HB2	1.61	0.81
1:A:377:THR:O	1:A:381:VAL:HG23	1.81	0.80
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.13	0.78
1:A:229:TRP:CE3	1:A:229:TRP:HA	2.19	0.78
2:B:421:PRO:O	2:B:425:LEU:HD22	1.85	0.77
2:B:92:LEU:HD13	2:B:161:GLN:HB3	1.66	0.76
1:A:229:TRP:HE3	1:A:229:TRP:HA	1.50	0.76
1:A:519:ASN:HA	1:A:522:ILE:HD12	1.67	0.76
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.66	0.75
1:A:208:HIS:O	1:A:211:ARG:HB2	1.87	0.75
1:A:356:ARG:NH2	1:A:367:GLN:O	2.21	0.74
1:A:181:TYR:CD1	2:B:138:GLU:HB3	2.22	0.74
2:B:379:SER:CB	2:B:387:PRO:HD3	2.19	0.73
1:A:309:ILE:O	1:A:312:GLU:HB3	1.88	0.73
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.71	0.73
2:B:178:ILE:HG12	2:B:191:SER:CB	2.16	0.73
2:B:266:TRP:HZ3	2:B:426:TRP:CG	2.06	0.73
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.07	0.73
2:B:60:VAL:HG21	2:B:130:PHE:HD2	1.54	0.72
1:A:241:VAL:HG21	1:A:314:VAL:HG23	1.72	0.72
1:A:8:VAL:O	1:A:121:ASP:HB2	1.89	0.72
1:A:465:LYS:HG3	1:A:466:VAL:N	2.05	0.71
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.70	0.71
2:B:254:VAL:HG22	2:B:293:ILE:HD11	1.71	0.71
2:B:328:GLU:O	2:B:339:TYR:HA	1.90	0.71
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.26	0.71
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.72	0.71
1:A:244:ILE:HD11	1:A:263:LYS:HE3	1.71	0.71
2:B:344:GLU:HG3	2:B:345:PRO:HD2	1.71	0.71
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.72	0.71
1:A:34:LEU:HD22	1:A:73:LYS:HG3	1.72	0.71
1:A:340:GLN:CB	1:A:351:THR:HG22	2.20	0.71
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.89	0.71
1:A:164:MET:HE1	1:A:214:LEU:HD23	1.73	0.70
1:A:356:ARG:HE	1:A:367:GLN:HG2	1.56	0.70
2:B:122:GLU:HG3	2:B:125:ARG:NH1	2.07	0.70
1:A:542:ILE:CG1	2:B:283:LEU:HD23	2.22	0.70
2:B:5:ILE:HG13	2:B:6:GLU:N	2.06	0.69
1:A:63:ILE:HD12	1:A:65:LYS:HE3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASN:O	1:A:478:GLU:HG3	1.92	0.69
2:B:215:THR:C	2:B:217:PRO:HD3	2.12	0.69
2:B:125:ARG:HG2	2:B:146:TYR:O	1.93	0.68
2:B:426:TRP:O	2:B:429:LEU:HB2	1.93	0.68
2:B:175:ASN:ND2	2:B:201:LYS:HE2	2.08	0.68
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.75	0.68
1:A:27:THR:HB	1:A:30:LYS:HG3	1.76	0.68
1:A:33:ALA:HB1	1:A:71:TRP:HB2	1.75	0.67
2:B:163:SER:O	2:B:167:ILE:HG13	1.95	0.67
1:A:517:LEU:O	1:A:521:ILE:HG13	1.95	0.67
2:B:266:TRP:CZ3	2:B:426:TRP:CG	2.83	0.67
1:A:362:THR:HG22	1:A:363:ASN:H	1.58	0.67
1:A:240:THR:HG22	1:A:315:HIS:HD2	1.59	0.66
2:B:158:ALA:O	2:B:161:GLN:HB2	1.96	0.66
1:A:28:GLU:CD	1:A:32:LYS:HE3	2.16	0.66
1:A:164:MET:HG3	1:A:168:LEU:HD22	1.79	0.65
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.78	0.64
1:A:114:ALA:HB1	1:A:214:LEU:HG	1.77	0.64
1:A:224:GLU:HG2	1:A:225:PRO:HD2	1.78	0.64
2:B:281:LYS:HD3	2:B:284:ARG:NH2	2.12	0.64
1:A:202:ILE:CG2	1:A:206:ARG:HH21	2.10	0.64
1:A:66:LYS:HD3	1:A:66:LYS:H	1.62	0.64
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.28	0.64
1:A:277:ARG:O	1:A:281:LYS:HG3	1.97	0.64
1:A:393:ILE:HG23	1:A:423:VAL:HG22	1.77	0.64
2:B:104:LYS:CB	2:B:192:ASP:HA	2.25	0.64
1:A:31:ILE:HD12	1:A:135:ILE:HD12	1.81	0.63
1:A:278:GLN:O	1:A:282:LEU:HD13	1.99	0.63
1:A:20:LYS:HD2	1:A:55:PRO:O	1.99	0.63
2:B:435:VAL:HG23	2:B:436:GLY:H	1.64	0.63
1:A:219:LYS:HE3	1:A:219:LYS:HA	1.80	0.63
1:A:78:ARG:HG3	1:A:79:GLU:N	2.11	0.63
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.80	0.62
1:A:7:THR:HG21	1:A:122:GLU:OE2	1.98	0.62
1:A:26:LEU:HD12	1:A:133:PRO:HD2	1.81	0.62
2:B:369:THR:O	2:B:373:GLN:HG3	1.99	0.62
2:B:434:ILE:HG13	2:B:435:VAL:HG22	1.82	0.62
1:A:253:THR:HG22	1:A:255:ASN:HB2	1.81	0.62
1:A:280:CSD:O	1:A:283:LEU:HB2	1.99	0.62
2:B:277:ARG:O	2:B:281:LYS:HG2	2.01	0.61
2:B:303:LEU:O	2:B:307:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:ILE:HG13	2:B:435:VAL:N	2.14	0.61
1:A:241:VAL:CG2	1:A:314:VAL:HG23	2.30	0.61
1:A:393:ILE:HD12	1:A:414:TRP:CZ3	2.36	0.61
2:B:78:ARG:O	2:B:82:LYS:HG3	1.99	0.61
1:A:252:TRP:CD1	1:A:295:LEU:HD21	2.36	0.61
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.35	0.61
2:B:50:ILE:HG13	2:B:143:ARG:HB3	1.83	0.61
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.14	0.61
1:A:101:LYS:HD3	1:A:321:PRO:HG2	1.82	0.61
1:A:400:THR:HG22	1:A:425:LEU:HD11	1.82	0.61
2:B:101:LYS:HE3	2:B:382:ILE:HA	1.83	0.61
2:B:175:ASN:HD21	2:B:201:LYS:HE2	1.65	0.61
1:A:373:GLN:HG2	3:B:1237:HOH:O	2.01	0.60
2:B:180:ILE:HG13	2:B:189:VAL:HG22	1.83	0.60
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.82	0.60
1:A:231:GLY:HA2	1:A:242:GLN:HB2	1.82	0.60
2:B:244:ILE:HG23	2:B:429:LEU:HB3	1.83	0.60
1:A:125:ARG:HG2	1:A:146:TYR:O	2.01	0.60
1:A:254:VAL:O	1:A:258:GLN:HG3	2.01	0.60
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.36	0.60
1:A:3:SER:HB3	1:A:4:PRO:HD2	1.84	0.60
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.84	0.59
2:B:31:ILE:O	2:B:35:VAL:HG23	2.01	0.59
2:B:301:LEU:HG	2:B:301:LEU:O	2.02	0.59
2:B:278:GLN:O	2:B:299:ALA:HB2	2.01	0.59
1:A:297:GLU:HG2	1:A:298:GLU:N	2.17	0.59
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.32	0.59
1:A:357:MET:O	1:A:358:ARG:HB3	2.02	0.59
1:A:113:ASP:HB2	3:A:1045:HOH:O	2.03	0.58
1:A:329:ILE:HD12	1:A:391:LEU:HD21	1.85	0.58
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.38	0.58
2:B:97:PRO:O	2:B:99:GLY:N	2.33	0.58
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.85	0.58
1:A:491:LEU:HD22	1:A:529:GLU:HG3	1.85	0.58
1:A:233:GLU:HB2	1:A:240:THR:OG1	2.03	0.58
1:A:27:THR:HG22	1:A:29:GLU:H	1.67	0.58
2:B:301:LEU:O	2:B:304:ALA:HB3	2.03	0.58
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.39	0.58
1:A:164:MET:CE	1:A:214:LEU:HD23	2.33	0.58
2:B:114:ALA:HB2	2:B:214:LEU:HG	1.85	0.58
2:B:64:LYS:HE3	2:B:71:TRP:NE1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD22	1:A:83:ARG:O	2.04	0.57
1:A:340:GLN:HA	1:A:351:THR:HA	1.86	0.57
2:B:379:SER:HB2	2:B:387:PRO:HD3	1.84	0.57
1:A:235:HIS:HB2	1:A:238:LYS:O	2.04	0.57
1:A:511:ASP:HA	1:A:522:ILE:HG21	1.85	0.57
2:B:282:LEU:HD11	2:B:295:LEU:HD23	1.86	0.57
2:B:328:GLU:HG3	2:B:390:LYS:HB2	1.87	0.57
1:A:31:ILE:HD12	1:A:135:ILE:CD1	2.34	0.57
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.39	0.57
2:B:254:VAL:O	2:B:258:GLN:HG3	2.05	0.57
1:A:317:VAL:HG12	1:A:349:LEU:HD23	1.87	0.56
1:A:95:PRO:HD3	1:A:183:TYR:CE2	2.40	0.56
1:A:438:GLU:CD	1:A:461:ARG:HD2	2.26	0.56
1:A:7:THR:CG2	1:A:121:ASP:HA	2.36	0.56
1:A:401:TRP:HZ3	1:A:409:THR:HG21	1.70	0.56
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.26	0.56
2:B:134:SER:CB	2:B:139:THR:HG23	2.36	0.56
2:B:108:VAL:HG13	2:B:188:TYR:CE1	2.41	0.56
2:B:366:LYS:O	2:B:370:GLU:HG3	2.05	0.56
1:A:28:GLU:HB3	3:A:1026:HOH:O	2.05	0.56
2:B:3:SER:O	2:B:119:PRO:HD3	2.05	0.55
1:A:27:THR:O	1:A:31:ILE:HG13	2.05	0.55
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.53	0.55
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.88	0.55
1:A:22:LYS:HG2	1:A:23:GLN:N	2.22	0.55
1:A:295:LEU:N	1:A:295:LEU:HD23	2.21	0.55
2:B:105:SER:O	2:B:190:GLY:HA2	2.07	0.55
1:A:200:THR:O	1:A:203:GLU:HB3	2.07	0.55
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.42	0.55
1:A:33:ALA:O	1:A:37:ILE:HG13	2.07	0.54
2:B:111:VAL:HG21	2:B:164:MET:CE	2.38	0.54
2:B:270:ILE:O	2:B:272:PRO:HD3	2.08	0.54
2:B:380:ILE:O	2:B:384:GLY:N	2.39	0.54
1:A:312:GLU:HG2	1:A:313:PRO:N	2.22	0.54
1:A:366:LYS:NZ	2:B:394:GLN:NE2	2.55	0.54
1:A:63:ILE:O	1:A:63:ILE:HG13	2.07	0.54
2:B:288:ALA:O	2:B:291:GLU:HB3	2.08	0.54
2:B:235:HIS:HB3	2:B:238:LYS:HG2	1.90	0.54
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.73	0.54
2:B:292:VAL:C	2:B:293:ILE:HG13	2.29	0.53
2:B:356:ARG:HB3	2:B:367:GLN:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:CD	1:A:122:GLU:H	2.12	0.53
1:A:26:LEU:HD12	1:A:133:PRO:CD	2.38	0.53
2:B:433:PRO:HG3	2:B:436:GLY:HA2	1.90	0.53
2:B:122:GLU:HG3	2:B:125:ARG:HH11	1.72	0.53
2:B:281:LYS:HD3	2:B:284:ARG:HH21	1.74	0.53
1:A:400:THR:CG2	1:A:425:LEU:HD11	2.37	0.53
1:A:239:TRP:CZ2	1:A:349:LEU:O	2.57	0.53
1:A:380:ILE:HG13	1:A:386:THR:HG22	1.90	0.53
2:B:134:SER:HB3	2:B:139:THR:HG23	1.90	0.53
1:A:490:GLY:O	1:A:528:LYS:HE3	2.09	0.53
1:A:361:HIS:CE1	1:A:510:PRO:HG3	2.43	0.52
1:A:241:VAL:HG21	1:A:270:ILE:HD12	1.91	0.52
1:A:218:ASP:O	1:A:222:GLN:HG2	2.09	0.52
1:A:218:ASP:O	1:A:219:LYS:HE3	2.09	0.52
2:B:319:TYR:HE1	2:B:325:LEU:HD13	1.74	0.52
1:A:197:GLN:O	1:A:200:THR:HB	2.09	0.52
2:B:118:VAL:HG21	2:B:160:PHE:HD1	1.75	0.52
2:B:200:THR:O	2:B:203:GLU:HB3	2.08	0.52
1:A:500:GLN:O	1:A:503:LEU:HB3	2.10	0.52
2:B:205:LEU:HD13	2:B:209:LEU:HD12	1.91	0.52
2:B:51:GLY:HA3	2:B:53:GLU:OE2	2.10	0.52
2:B:242:GLN:HE21	2:B:242:GLN:HA	1.75	0.52
2:B:281:LYS:HA	2:B:284:ARG:NH2	2.25	0.52
1:A:516:GLU:O	1:A:519:ASN:HB2	2.11	0.51
2:B:125:ARG:O	2:B:128:THR:OG1	2.23	0.51
1:A:307:ARG:O	1:A:311:LYS:HG3	2.09	0.51
1:A:519:ASN:O	1:A:523:GLU:HG2	2.10	0.51
1:A:517:LEU:HA	1:A:520:GLN:CG	2.41	0.51
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.93	0.51
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.45	0.51
2:B:424:LYS:O	2:B:424:LYS:HD2	2.10	0.51
2:B:92:LEU:HD13	2:B:161:GLN:CB	2.37	0.51
2:B:100:LEU:O	2:B:103:LYS:HB2	2.11	0.51
1:A:255:ASN:HB3	1:A:259:LYS:HE2	1.92	0.50
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.41	0.50
1:A:532:TYR:HE2	1:A:534:ALA:HB2	1.76	0.50
2:B:245:VAL:CG1	2:B:431:LYS:HB2	2.41	0.50
2:B:329:ILE:HA	2:B:338:THR:O	2.11	0.50
2:B:362:THR:O	2:B:362:THR:HG22	2.12	0.50
2:B:311:LYS:O	2:B:312:GLU:HG3	2.12	0.50
2:B:54:ASN:O	2:B:143:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HG23	1:A:119:PRO:HD2	1.93	0.50
1:A:11:LYS:O	1:A:85:GLN:HB3	2.12	0.50
1:A:35:VAL:HG22	1:A:132:ILE:HG21	1.94	0.50
2:B:326:ILE:HG22	2:B:327:ALA:N	2.27	0.50
1:A:206:ARG:O	1:A:210:LEU:HD23	2.12	0.50
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.46	0.50
2:B:23:GLN:HG3	2:B:24:TRP:O	2.12	0.50
1:A:229:TRP:O	1:A:230:MET:HG3	2.11	0.50
1:A:67:ASP:HB2	1:A:72:ARG:HH12	1.77	0.50
1:A:149:LEU:HD13	1:A:156:SER:HA	1.93	0.49
1:A:111:VAL:HG11	1:A:187:LEU:CD2	2.42	0.49
1:A:334:GLN:NE2	3:A:1091:HOH:O	2.42	0.49
1:A:362:THR:O	1:A:510:PRO:HA	2.12	0.49
2:B:22:LYS:HD3	2:B:22:LYS:H	1.76	0.49
2:B:94:ILE:HG13	2:B:95:PRO:HD2	1.94	0.49
2:B:17:ASP:O	2:B:83:ARG:HD3	2.12	0.49
2:B:215:THR:O	2:B:217:PRO:HD3	2.12	0.49
1:A:362:THR:CG2	1:A:363:ASN:H	2.20	0.49
1:A:463:ARG:NH1	1:A:488:ASP:O	2.45	0.49
1:A:486:LEU:HB3	1:A:524:GLN:HB3	1.94	0.49
2:B:249:LYS:HG2	2:B:252:TRP:CE2	2.48	0.49
2:B:162:SER:O	2:B:166:LYS:HG3	2.11	0.49
2:B:36:GLU:O	2:B:39:THR:HG22	2.12	0.49
2:B:79:GLU:O	2:B:83:ARG:HG3	2.13	0.49
1:A:231:GLY:CA	1:A:242:GLN:HB2	2.43	0.49
1:A:34:LEU:HD23	1:A:37:ILE:HD12	1.95	0.49
1:A:7:THR:HG21	1:A:121:ASP:HA	1.95	0.49
1:A:240:THR:HG22	1:A:315:HIS:CD2	2.43	0.49
1:A:78:ARG:CG	1:A:79:GLU:N	2.74	0.49
2:B:78:ARG:HH11	2:B:411:ILE:CG2	2.26	0.49
1:A:393:ILE:HD12	1:A:414:TRP:CH2	2.48	0.49
2:B:169:GLU:O	2:B:173:LYS:N	2.46	0.49
2:B:85:GLN:O	2:B:85:GLN:HG2	2.12	0.49
1:A:218:ASP:O	1:A:222:GLN:CG	2.60	0.49
1:A:13:LYS:O	1:A:16:MET:HB2	2.12	0.49
2:B:363:ASN:ND2	2:B:405:TYR:OH	2.41	0.48
1:A:253:THR:O	1:A:257:ILE:HG13	2.12	0.48
1:A:486:LEU:O	1:A:528:LYS:NZ	2.45	0.48
2:B:261:VAL:HG22	2:B:276:VAL:HG22	1.96	0.48
2:B:319:TYR:CZ	2:B:321:PRO:HA	2.48	0.48
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:HB3	1:A:16:MET:SD	2.53	0.48
1:A:73:LYS:HB3	1:A:73:LYS:NZ	2.28	0.48
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.61	0.48
2:B:422:LEU:HB2	3:B:1244:HOH:O	2.12	0.48
1:A:5:ILE:HG23	1:A:119:PRO:CD	2.44	0.48
1:A:122:GLU:HA	1:A:125:ARG:NE	2.29	0.48
1:A:27:THR:HG22	1:A:29:GLU:N	2.28	0.48
1:A:3:SER:CB	1:A:5:ILE:HG22	2.43	0.48
1:A:111:VAL:HG11	1:A:187:LEU:HD22	1.96	0.48
1:A:37:ILE:HD11	1:A:71:TRP:O	2.13	0.48
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.14	0.48
1:A:303:LEU:HD11	1:A:307:ARG:NH2	2.29	0.48
1:A:536:VAL:HG11	1:A:542:ILE:HG21	1.95	0.48
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.95	0.48
1:A:305:GLU:O	1:A:308:GLU:HB2	2.13	0.48
2:B:65:LYS:N	2:B:68:SER:HB2	2.29	0.48
1:A:103:LYS:HG3	1:A:190:GLY:C	2.35	0.47
2:B:120:LEU:HD12	2:B:150:PRO:HD3	1.96	0.47
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.44	0.47
2:B:111:VAL:HG21	2:B:164:MET:HE2	1.97	0.47
2:B:169:GLU:O	2:B:173:LYS:HB2	2.15	0.47
2:B:379:SER:HA	2:B:383:TRP:CE3	2.49	0.47
2:B:398:TRP:O	2:B:402:TRP:HD1	1.98	0.47
2:B:8:VAL:HG13	2:B:159:ILE:HD13	1.96	0.47
2:B:350:LYS:HG2	2:B:351:THR:N	2.29	0.47
2:B:29:GLU:HG3	2:B:71:TRP:CZ2	2.49	0.47
1:A:356:ARG:HH21	1:A:367:GLN:CA	2.28	0.47
1:A:448:ARG:HB3	3:A:1154:HOH:O	2.15	0.47
2:B:435:VAL:HG23	2:B:436:GLY:N	2.29	0.47
1:A:220:LYS:HB3	1:A:221:HIS:CE1	2.50	0.47
2:B:153:TRP:HE3	2:B:156:SER:OG	1.98	0.47
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.97	0.47
1:A:448:ARG:HB2	1:A:448:ARG:NH1	2.30	0.47
2:B:191:SER:HB2	2:B:193:LEU:HD23	1.96	0.47
2:B:213:GLY:O	2:B:214:LEU:HB3	2.15	0.47
2:B:338:THR:HG22	2:B:353:LYS:HD3	1.96	0.47
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.50	0.47
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.50	0.47
1:A:229:TRP:CB	1:A:232:TYR:HB2	2.40	0.46
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.51	0.46
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:TRP:CE3	2:B:256:ASP:HB3	2.50	0.46
2:B:379:SER:HA	2:B:383:TRP:HE3	1.80	0.46
1:A:498:ASP:HA	1:A:536:VAL:O	2.16	0.46
2:B:327:ALA:O	2:B:389:PHE:HA	2.16	0.46
2:B:34:LEU:O	2:B:38:CYS:HB2	2.15	0.46
1:A:115:TYR:OH	1:A:151:GLN:HB2	2.14	0.46
1:A:517:LEU:HA	1:A:520:GLN:HG3	1.98	0.46
2:B:254:VAL:HG12	2:B:258:GLN:NE2	2.30	0.46
2:B:319:TYR:CE1	2:B:325:LEU:HD13	2.50	0.46
1:A:28:GLU:O	1:A:32:LYS:HG3	2.14	0.46
1:A:500:GLN:O	1:A:503:LEU:CB	2.64	0.46
2:B:379:SER:HB3	2:B:387:PRO:HD3	1.98	0.46
1:A:360:ALA:HA	1:A:514:GLU:HB2	1.98	0.46
2:B:380:ILE:O	2:B:384:GLY:HA2	2.15	0.46
2:B:61:PHE:HB2	2:B:74:LEU:HD23	1.98	0.46
1:A:489:SER:CB	1:A:493:VAL:HG13	2.46	0.46
2:B:261:VAL:HG22	2:B:276:VAL:CG2	2.46	0.46
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.97	0.46
1:A:328:GLU:O	1:A:339:TYR:HA	2.16	0.45
1:A:380:ILE:CG1	1:A:386:THR:HG22	2.46	0.45
1:A:542:ILE:HD12	1:A:542:ILE:N	2.31	0.45
2:B:196:GLY:O	2:B:200:THR:HG23	2.17	0.45
1:A:469:LEU:HB2	1:A:472:THR:HG21	1.97	0.45
2:B:183:TYR:HB3	2:B:188:TYR:HE2	1.80	0.45
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.81	0.45
2:B:376:THR:CG2	2:B:386:THR:HG22	2.46	0.45
2:B:5:ILE:CG1	2:B:6:GLU:N	2.74	0.45
1:A:401:TRP:HB2	1:A:425:LEU:HD21	1.98	0.45
2:B:253:THR:H	2:B:256:ASP:HB2	1.81	0.45
2:B:406:TRP:CZ2	2:B:412:PRO:HD2	2.52	0.45
2:B:97:PRO:C	2:B:99:GLY:H	2.17	0.45
1:A:94:ILE:HG22	1:A:95:PRO:O	2.16	0.45
2:B:60:VAL:CG2	2:B:130:PHE:HD2	2.26	0.45
2:B:271:TYR:O	2:B:274:ILE:HG12	2.16	0.45
2:B:334:GLN:HA	2:B:334:GLN:OE1	2.16	0.45
2:B:369:THR:CG2	2:B:398:TRP:CH2	3.00	0.45
1:A:515:SER:CB	1:A:518:VAL:HG23	2.45	0.45
2:B:118:VAL:HB	2:B:149:LEU:HG	1.97	0.45
2:B:359:GLY:O	2:B:361:HIS:N	2.50	0.45
2:B:120:LEU:HD21	2:B:124:PHE:HB3	1.98	0.45
2:B:259:LYS:HE3	3:B:1217:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:TRP:O	2:B:410:TRP:CE3	2.70	0.44
1:A:222:GLN:CD	1:A:223:LYS:H	2.21	0.44
1:A:267:ALA:O	1:A:269:GLN:N	2.50	0.44
1:A:326:ILE:O	1:A:341:ILE:HG23	2.17	0.44
1:A:478:GLU:O	1:A:481:ALA:HB3	2.17	0.44
1:A:254:VAL:HG23	1:A:291:GLU:O	2.16	0.44
2:B:249:LYS:HB3	2:B:249:LYS:HE3	1.66	0.44
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.99	0.44
1:A:431:LYS:HD3	1:A:431:LYS:HA	1.47	0.44
2:B:248:GLU:HG3	2:B:248:GLU:O	2.18	0.44
1:A:323:LYS:HB3	1:A:343:GLN:NE2	2.32	0.44
1:A:73:LYS:HE2	1:A:75:VAL:HG23	1.98	0.44
2:B:174:GLN:HA	2:B:174:GLN:HE21	1.83	0.44
2:B:266:TRP:O	2:B:269:GLN:OE1	2.35	0.44
2:B:433:PRO:CG	2:B:436:GLY:HA2	2.47	0.44
1:A:210:LEU:HA	1:A:210:LEU:HD13	1.65	0.44
1:A:224:GLU:HG2	1:A:225:PRO:CD	2.47	0.44
1:A:73:LYS:HE2	1:A:75:VAL:CG2	2.48	0.44
2:B:195:ILE:O	2:B:199:ARG:HG3	2.18	0.44
2:B:65:LYS:HE3	2:B:72:ARG:HG2	2.00	0.44
1:A:229:TRP:CE3	1:A:229:TRP:CA	2.98	0.44
1:A:483:TYR:CE2	1:A:487:GLN:OE1	2.70	0.44
2:B:235:HIS:N	2:B:236:PRO:HD3	2.32	0.44
1:A:50:ILE:HG21	1:A:145:GLN:HG2	1.98	0.44
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.81	0.44
1:A:386:THR:HA	1:A:387:PRO:HD2	1.62	0.43
2:B:118:VAL:HG21	2:B:160:PHE:CD1	2.52	0.43
2:B:174:GLN:O	2:B:176:PRO:HD3	2.17	0.43
2:B:198:HIS:O	2:B:202:ILE:HG12	2.18	0.43
1:A:34:LEU:HA	1:A:37:ILE:HD12	1.99	0.43
1:A:366:LYS:O	1:A:369:THR:HB	2.18	0.43
2:B:176:PRO:HA	3:B:1209:HOH:O	2.18	0.43
2:B:61:PHE:CD1	2:B:403:THR:HG21	2.53	0.43
1:A:65:LYS:C	1:A:67:ASP:H	2.22	0.43
2:B:96:HIS:HE1	2:B:100:LEU:HD21	1.83	0.43
2:B:209:LEU:O	2:B:214:LEU:HD13	2.18	0.43
2:B:60:VAL:HG21	2:B:130:PHE:CD2	2.43	0.43
1:A:22:LYS:HG2	1:A:23:GLN:H	1.81	0.43
1:A:540:LYS:HB2	1:A:542:ILE:HD13	2.01	0.43
1:A:31:ILE:HD13	1:A:133:PRO:O	2.18	0.43
1:A:229:TRP:O	1:A:232:TYR:CD2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:HA	1:A:135:ILE:HD11	2.00	0.43
1:A:80:LEU:HD12	1:A:80:LEU:O	2.19	0.43
2:B:271:TYR:HB3	2:B:309:ILE:CG2	2.49	0.43
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.43
1:A:347:LYS:HD2	3:A:1108:HOH:O	2.17	0.43
2:B:87:PHE:CE2	2:B:154:LYS:HE3	2.53	0.43
2:B:379:SER:O	2:B:385:LYS:O	2.37	0.43
2:B:325:LEU:HA	2:B:343:GLN:HG2	2.00	0.43
2:B:379:SER:OG	2:B:387:PRO:HG3	2.19	0.43
1:A:231:GLY:O	1:A:242:GLN:N	2.50	0.43
2:B:206:ARG:HB3	2:B:206:ARG:NH1	2.34	0.43
1:A:257:ILE:O	1:A:261:VAL:HG23	2.19	0.43
1:A:420:PRO:HA	1:A:421:PRO:C	2.38	0.43
1:A:497:THR:O	1:A:535:TRP:HA	2.19	0.43
1:A:34:LEU:CD2	1:A:73:LYS:HG3	2.47	0.43
1:A:65:LYS:HD2	1:A:65:LYS:HA	1.93	0.42
2:B:393:ILE:HD13	2:B:398:TRP:HB2	2.00	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.18	0.42
2:B:267:ALA:C	2:B:269:GLN:H	2.21	0.42
2:B:271:TYR:HB3	2:B:309:ILE:HG21	2.01	0.42
1:A:31:ILE:CD1	1:A:135:ILE:HD12	2.46	0.42
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.77	0.42
2:B:156:SER:O	2:B:158:ALA:N	2.52	0.42
2:B:424:LYS:C	2:B:424:LYS:HD2	2.39	0.42
1:A:3:SER:HB2	1:A:5:ILE:HG22	2.00	0.42
1:A:118:VAL:HB	1:A:149:LEU:HG	2.02	0.42
1:A:3:SER:HB3	1:A:5:ILE:HG22	2.01	0.42
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.54	0.42
2:B:363:ASN:ND2	2:B:405:TYR:CZ	2.87	0.42
1:A:345:PRO:C	1:A:347:LYS:H	2.23	0.42
1:A:3:SER:HB2	1:A:5:ILE:CG2	2.49	0.42
1:A:61:PHE:HE2	1:A:76:ASP:OD2	2.03	0.42
2:B:303:LEU:HA	2:B:303:LEU:HD23	1.88	0.42
2:B:50:ILE:CG2	2:B:145:GLN:HB2	2.50	0.42
1:A:20:LYS:NZ	1:A:20:LYS:HB2	2.33	0.42
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.54	0.42
1:A:366:LYS:HZ3	2:B:394:GLN:HE21	1.68	0.42
1:A:208:HIS:HE1	1:A:212:TRP:HE1	1.60	0.42
1:A:454:LYS:HA	1:A:467:VAL:O	2.19	0.42
2:B:120:LEU:HD23	2:B:120:LEU:C	2.40	0.42
1:A:181:TYR:CE1	2:B:138:GLU:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:CG2	1:A:206:ARG:NH2	2.82	0.42
1:A:417:VAL:O	1:A:417:VAL:HG13	2.20	0.42
2:B:242:GLN:NE2	2:B:243:PRO:HD2	2.34	0.42
2:B:380:ILE:O	2:B:384:GLY:CA	2.68	0.42
1:A:136:ASN:HD22	1:A:136:ASN:C	2.23	0.42
1:A:279:LEU:HD23	1:A:302:GLU:OE2	2.20	0.42
1:A:521:ILE:O	1:A:525:LEU:HG	2.20	0.42
1:A:89:GLU:OE2	1:A:91:GLN:HB2	2.19	0.42
1:A:389:PHE:HB2	1:A:414:TRP:HB3	2.01	0.41
2:B:26:LEU:HD13	2:B:31:ILE:HD13	2.01	0.41
1:A:341:ILE:N	1:A:350:LYS:O	2.49	0.41
1:A:517:LEU:HA	1:A:520:GLN:HG2	2.01	0.41
1:A:155:GLY:O	1:A:156:SER:C	2.58	0.41
1:A:26:LEU:HG	1:A:133:PRO:HG2	2.02	0.41
1:A:379:SER:HA	1:A:383:TRP:CE3	2.54	0.41
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.29	0.41
1:A:8:VAL:HG21	1:A:159:ILE:HG12	2.02	0.41
1:A:504:GLY:O	1:A:507:GLN:N	2.54	0.41
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.55	0.41
1:A:253:THR:HB	1:A:256:ASP:OD2	2.19	0.41
1:A:520:GLN:HG2	1:A:520:GLN:H	1.66	0.41
1:A:64:LYS:HB2	1:A:71:TRP:CH2	2.56	0.41
2:B:252:TRP:HE3	2:B:256:ASP:HB3	1.84	0.41
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.96	0.41
1:A:465:LYS:HG3	1:A:466:VAL:H	1.81	0.41
1:A:516:GLU:O	1:A:520:GLN:HG2	2.21	0.41
2:B:103:LYS:HD3	2:B:103:LYS:HA	1.79	0.41
2:B:120:LEU:HD22	2:B:125:ARG:HG3	2.02	0.41
2:B:349:LEU:HD23	2:B:349:LEU:HA	1.84	0.41
1:A:220:LYS:HE3	1:A:221:HIS:NE2	2.35	0.41
1:A:238:LYS:HA	1:A:316:GLY:O	2.20	0.41
1:A:358:ARG:HG2	1:A:358:ARG:O	2.20	0.41
1:A:420:PRO:HB3	1:A:421:PRO:HA	2.01	0.41
1:A:520:GLN:O	1:A:523:GLU:HB2	2.21	0.41
1:A:121:ASP:N	3:A:1012:HOH:O	2.54	0.41
1:A:23:GLN:HG3	1:A:133:PRO:HG3	2.03	0.41
2:B:174:GLN:CA	2:B:174:GLN:HE21	2.32	0.41
2:B:216:THR:N	2:B:217:PRO:HD3	2.36	0.41
2:B:354:TYR:CD1	2:B:354:TYR:C	2.94	0.41
2:B:65:LYS:HB2	2:B:68:SER:OG	2.21	0.41
1:A:77:PHE:HB2	1:A:152:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:SER:HA	1:A:383:TRP:HE3	1.84	0.41
1:A:60:VAL:HG23	1:A:75:VAL:HG22	2.02	0.41
2:B:22:LYS:HE2	2:B:22:LYS:HB2	1.93	0.41
1:A:286:THR:HG22	1:A:293:ILE:HD11	2.02	0.41
1:A:297:GLU:O	1:A:300:GLU:HB2	2.21	0.41
1:A:309:ILE:HG12	1:A:309:ILE:H	1.70	0.41
2:B:92:LEU:CD1	2:B:161:GLN:HB3	2.44	0.41
2:B:326:ILE:O	2:B:341:ILE:HA	2.21	0.41
2:B:431:LYS:HG2	2:B:432:GLU:N	2.36	0.41
1:A:135:ILE:HG22	1:A:136:ASN:N	2.36	0.41
1:A:225:PRO:HA	1:A:226:PRO:C	2.41	0.41
2:B:320:ASP:HA	2:B:321:PRO:HD2	1.88	0.41
2:B:361:HIS:HD1	2:B:361:HIS:C	2.23	0.41
1:A:173:LYS:HE2	1:A:173:LYS:HB3	1.91	0.40
2:B:174:GLN:O	2:B:174:GLN:NE2	2.54	0.40
2:B:206:ARG:HG2	2:B:216:THR:HB	2.04	0.40
2:B:342:TYR:HB3	2:B:348:ASN:HA	2.03	0.40
2:B:77:PHE:O	2:B:80:LEU:N	2.51	0.40
1:A:219:LYS:HA	1:A:219:LYS:CE	2.51	0.40
1:A:453:GLY:O	1:A:469:LEU:N	2.49	0.40
1:A:491:LEU:O	1:A:528:LYS:HB3	2.21	0.40
2:B:50:ILE:HG23	2:B:145:GLN:HB2	2.04	0.40
2:B:341:ILE:HD12	2:B:341:ILE:N	2.36	0.40
1:A:5:ILE:CD1	1:A:166:LYS:HD2	2.52	0.40
2:B:5:ILE:HG12	2:B:119:PRO:HD2	2.02	0.40
1:A:84:THR:O	1:A:85:GLN:O	2.38	0.40
2:B:145:GLN:NE2	3:B:1175:HOH:O	2.54	0.40
2:B:246:LEU:HD12	2:B:307:ARG:HG2	2.03	0.40
2:B:47:ILE:HB	2:B:145:GLN:O	2.21	0.40
1:A:57:ASN:ND2	1:A:58:THR:N	2.70	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	540/560 (96%)	458 (85%)	65 (12%)	17 (3%)	5	2
2	B	422/440 (96%)	365 (86%)	44 (10%)	13 (3%)	5	2
All	All	962/1000 (96%)	823 (86%)	109 (11%)	30 (3%)	5	2

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	85	GLN
2	B	98	ALA
1	A	14	PRO
1	A	268	SER
2	B	114	ALA
2	B	360	ALA
2	B	438	GLU
1	A	66	LYS
1	A	91	GLN
1	A	399	GLU
2	B	65	LYS
2	B	213	GLY
1	A	112	GLY
1	A	229	TRP
1	A	247	PRO
1	A	313	PRO
1	A	505	ILE
2	B	5	ILE
1	A	176	PRO
2	B	4	PRO
2	B	91	GLN
2	B	214	LEU
2	B	430	GLU
1	A	122	GLU
1	A	236	PRO
2	B	356	ARG
1	A	235	HIS
1	A	93	GLY
2	B	381	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/499 (97%)	402 (83%)	83 (17%)	2	1
2	B	386/400 (96%)	333 (86%)	53 (14%)	4	4
All	All	871/899 (97%)	735 (84%)	136 (16%)	3	2

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	14	PRO
1	A	16	MET
1	A	20	LYS
1	A	21	VAL
1	A	39	THR
1	A	41	MET
1	A	65	LYS
1	A	66	LYS
1	A	68	SER
1	A	69	THR
1	A	70	LYS
1	A	73	LYS
1	A	78	ARG
1	A	80	LEU
1	A	83	ARG
1	A	89	GLU
1	A	92	LEU
1	A	97	PRO
1	A	102	LYS
1	A	116	PHE
1	A	122	GLU
1	A	136	ASN
1	A	148	VAL
1	A	168	LEU
1	A	174	GLN

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Mol	Chain	Res	Type
1	A	182	GLN
1	A	185	ASP
1	A	186	ASP
1	A	187	LEU
1	A	195	ILE
1	A	208	HIS
1	A	210	LEU
1	A	211	ARG
1	A	219	LYS
1	A	221	HIS
1	A	222	GLN
1	A	229	TRP
1	A	230	MET
1	A	245	VAL
1	A	253	THR
1	A	263	LYS
1	A	264	LEU
1	A	276	VAL
1	A	282	LEU
1	A	283	LEU
1	A	295	LEU
1	A	297	GLU
1	A	303	LEU
1	A	312	GLU
1	A	314	VAL
1	A	323	LYS
1	A	325	LEU
1	A	330	GLN
1	A	331	LYS
1	A	332	GLN
1	A	334	GLN
1	A	340	GLN
1	A	348	ASN
1	A	356	ARG
1	A	362	THR
1	A	368	LEU
1	A	369	THR
1	A	373	GLN
1	A	388	LYS
1	A	393	ILE
1	A	400	THR
1	A	418	ASN

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Mol	Chain	Res	Type
1	A	419	THR
1	A	420	PRO
1	A	423	VAL
1	A	424	LYS
1	A	428	GLN
1	A	431	LYS
1	A	459	THR
1	A	465	LYS
1	A	474	ASN
1	A	493	VAL
1	A	515	SER
1	A	517	LEU
1	A	528	LYS
1	A	533	LEU
2	B	5	ILE
2	B	8	VAL
2	B	22	LYS
2	B	26	LEU
2	B	29	GLU
2	B	39	THR
2	B	53	GLU
2	B	69	THR
2	B	70	LYS
2	B	85	GLN
2	B	92	LEU
2	B	101	LYS
2	B	109	LEU
2	B	113	ASP
2	B	116	PHE
2	B	139	THR
2	B	163	SER
2	B	164	MET
2	B	165	THR
2	B	173	LYS
2	B	174	GLN
2	B	186	ASP
2	B	192	ASP
2	B	194	GLU
2	B	195	ILE
2	B	211	ARG
2	B	212	TRP
2	B	214	LEU

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Mol	Chain	Res	Type
2	B	216	THR
2	B	233	GLU
2	B	241	VAL
2	B	242	GLN
2	B	243	PRO
2	B	245	VAL
2	B	249	LYS
2	B	277	ARG
2	B	283	LEU
2	B	291	GLU
2	B	301	LEU
2	B	314	VAL
2	B	317	VAL
2	B	334	GLN
2	B	347	LYS
2	B	353	LYS
2	B	354	TYR
2	B	361	HIS
2	B	368	LEU
2	B	392	PRO
2	B	405	TYR
2	B	409	THR
2	B	424	LYS
2	B	425	LEU
2	B	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	197	GLN
1	A	208	HIS
1	A	235	HIS
1	A	242	GLN
1	A	278	GLN
1	A	315	HIS
1	A	330	GLN
1	A	334	GLN
1	A	340	GLN
1	A	363	ASN
1	A	418	ASN
1	A	474	ASN

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Mol	Chain	Res	Type
1	A	487	GLN
1	A	524	GLN
2	B	57	ASN
2	B	85	GLN
2	B	137	ASN
2	B	145	GLN
2	B	147	ASN
2	B	161	GLN
2	B	174	GLN
2	B	175	ASN
2	B	242	GLN
2	B	269	GLN
2	B	278	GLN
2	B	394	GLN
2	B	418	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	4,7,8	2.51	2 (50%)	2,8,10	7.72	2 (100%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	CB-SG	2.01	1.90	1.79
1	A	280	CSD	CA-C	4.38	1.56	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	O-C-CA	-2.02	119.44	125.02
1	A	280	CSD	OD1-SG-CB	10.73	125.73	105.61

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 1 short contact:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.