



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:29 am GMT

PDB ID : 1S6Q  
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN  
COMPLEX WITH JANSSEN-R147681  
Authors : Das, K.; Arnold, E.  
Deposited on : 2004-01-26  
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](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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

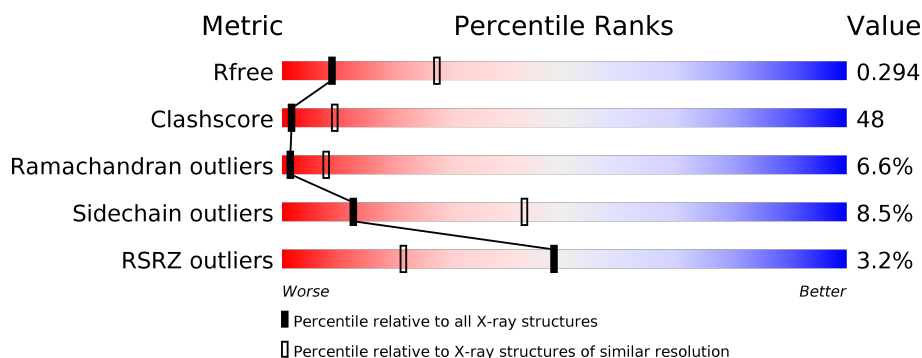
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	<div> <div>3%</div> <div> <div></div> <div>31%</div> <div>58%</div> <div>9%</div> </div> <div>•</div> </div>
2	B	430	<div> <div>3%</div> <div> <div></div> <div>38%</div> <div>50%</div> <div>10%</div> </div> <div>••</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	TPB	A	701	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8052 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 POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	61	0	0
			4498	2913	748	830	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	ENGINEERED	UNP P03366

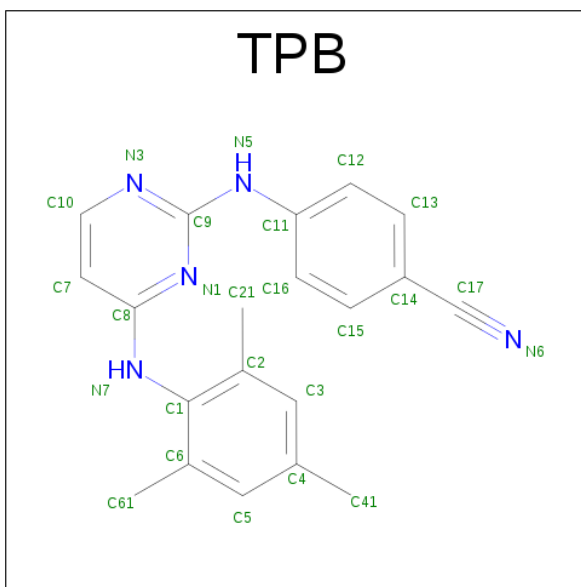
- Molecule 2 is a protein called POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	24	0	0
			3529	2300	584	638	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is 4-[4-(2,4,6-TRIMETHYL-PHENYLAMINO)-PYRIMIDIN-2-YLAMINO]-BE NZONITRILE (three-letter code: TPB) (formula: C<sub>20</sub>H<sub>19</sub>N<sub>5</sub>).

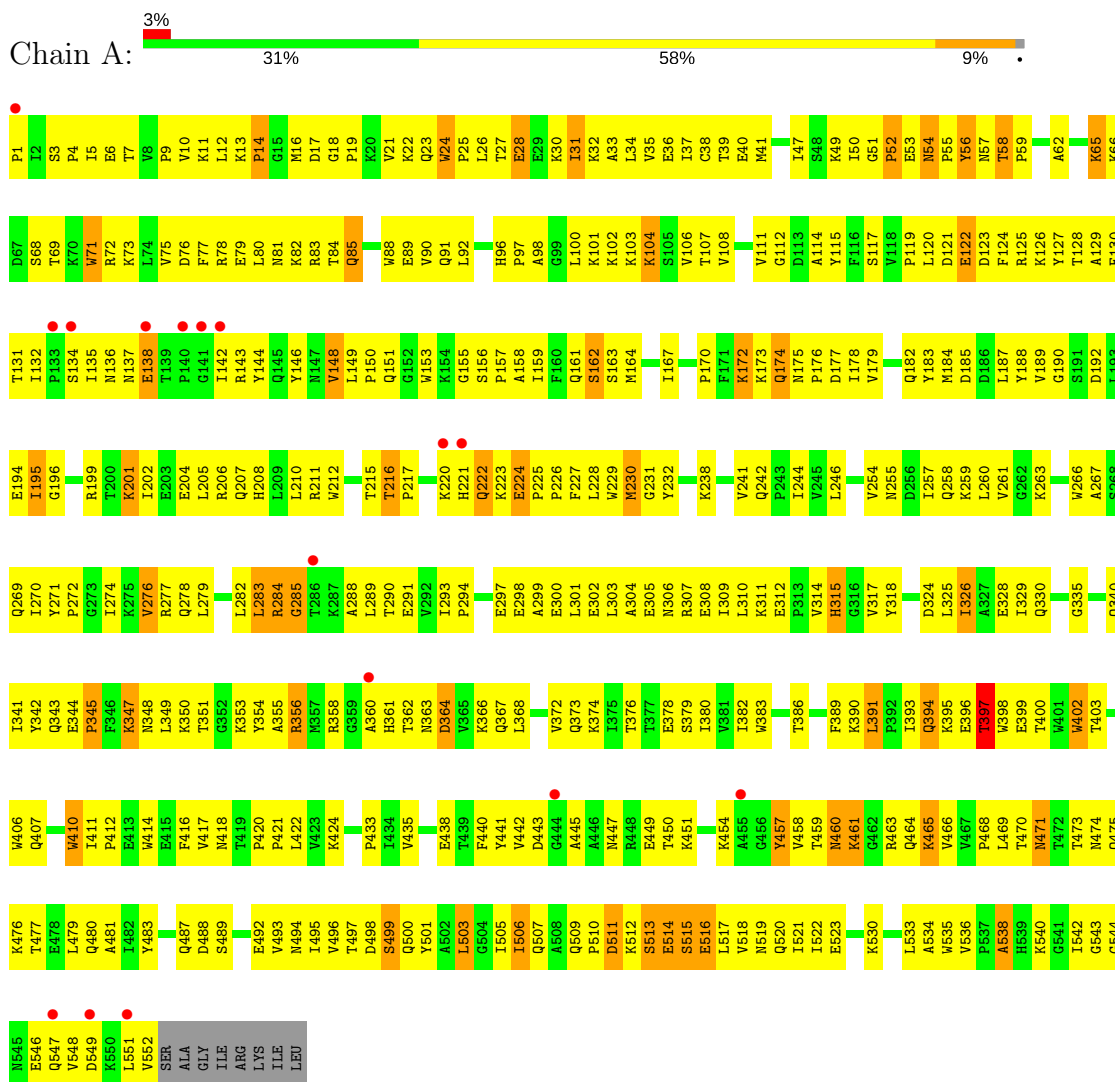


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			25	20	5		

### 3 Residue-property plots

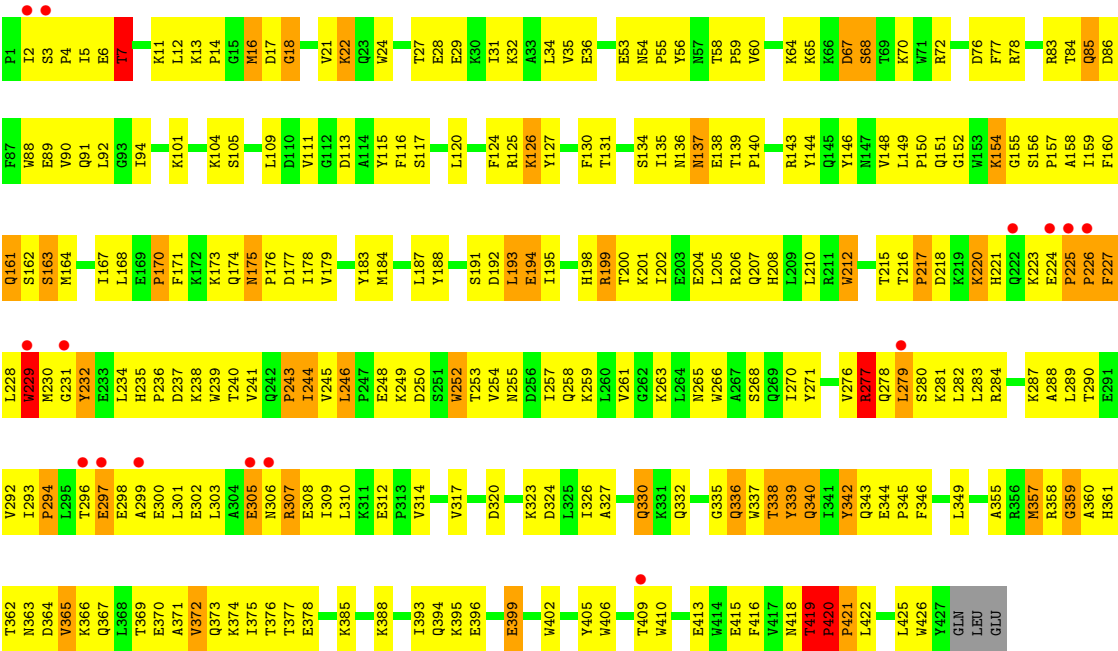
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: POL polyprotein [Contains: Reverse transcriptase]



- Molecule 2: POL polyprotein [Contains: Reverse transcriptase]





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.30Å 69.60Å 105.30Å 90.00° 106.30° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 35.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.6 (20.00-3.00) 94.8 (35.09-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.246 , 0.294 0.250 , 0.294	Depositor DCC
$R_{free}$ test set	1538 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.0	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 78.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

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	1/4616 (0.0%)	0.80	2/6271 (0.0%)
2	B	0.69	0/3634	0.89	5/4940 (0.1%)
All	All	0.63	1/8250 (0.0%)	0.84	7/11211 (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	1
2	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	GLU	CB-CG	5.02	1.61	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ASN	N-CA-C	7.32	130.76	111.00
2	B	419	THR	N-CA-C	6.25	127.88	111.00
2	B	225	PRO	N-CA-C	5.98	127.65	112.10
2	B	226	PRO	N-CA-C	-5.98	96.56	112.10
2	B	78	ARG	NE-CZ-NH2	-5.51	117.54	120.30
2	B	420	PRO	N-CA-C	5.43	126.22	112.10
1	A	285	GLY	N-CA-C	-5.34	99.74	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	TYR	Sidechain
2	B	188	TYR	Sidechain
2	B	339	TYR	Sidechain

## 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	4498	0	4560	470	0
2	B	3529	0	3568	326	0
3	A	25	0	19	5	0
All	All	8052	0	8147	768	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 48.

All (768) 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:454:LYS:HD2	1:A:552:VAL:HA	1.21	1.11
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.17	1.10
2:B:22:LYS:HE2	2:B:22:LYS:HA	1.36	1.06
2:B:357:MET:HB2	2:B:361:HIS:CE1	1.94	1.02
1:A:460:ASN:HD22	1:A:461:LYS:N	1.57	1.01
1:A:494:ASN:HD22	2:B:289:LEU:HD12	1.23	1.01
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.40	1.01
1:A:454:LYS:CD	1:A:552:VAL:HA	1.91	1.00
1:A:548:VAL:HA	1:A:551:LEU:HD12	1.40	0.99
2:B:357:MET:HB2	2:B:361:HIS:HE1	1.26	0.99
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.42	0.99
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.26	0.99
2:B:201:LYS:NZ	2:B:204:GLU:HG2	1.78	0.97
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.47	0.97
1:A:540:LYS:HD2	2:B:265:ASN:HD21	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:HA	2:B:281:LYS:HE3	1.47	0.96
1:A:298:GLU:H	1:A:298:GLU:CD	1.71	0.94
1:A:422:LEU:HD23	1:A:424:LYS:HD3	1.50	0.94
2:B:139:THR:CG2	2:B:140:PRO:HD2	1.96	0.94
2:B:263:LYS:HE3	2:B:425:LEU:HB3	1.47	0.94
1:A:288:ALA:HB1	1:A:291:GLU:HB3	1.45	0.93
1:A:90:VAL:HG23	1:A:91:GLN:HG2	1.51	0.93
1:A:315:HIS:NE2	1:A:347:LYS:HD3	1.83	0.92
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.34	0.92
1:A:460:ASN:ND2	1:A:461:LYS:H	1.68	0.91
2:B:241:VAL:HG12	2:B:243:PRO:HD3	1.48	0.91
1:A:100:LEU:HD21	3:A:701:TPB:H212	1.53	0.91
1:A:222:GLN:HG2	1:A:223:LYS:H	1.31	0.91
1:A:460:ASN:HD22	1:A:461:LYS:H	0.90	0.90
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.18	0.90
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.37	0.89
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.36	0.89
2:B:362:THR:CG2	2:B:367:GLN:HE21	1.84	0.89
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.56	0.88
1:A:543:GLY:HA3	2:B:284:ARG:HH11	1.39	0.88
1:A:106:VAL:HG12	1:A:107:THR:H	1.38	0.88
2:B:255:ASN:O	2:B:258:GLN:HB2	1.74	0.88
1:A:53:GLU:H	1:A:55:PRO:HD3	1.39	0.87
2:B:101:LYS:O	2:B:236:PRO:HB2	1.75	0.87
2:B:2:ILE:O	2:B:4:PRO:HD3	1.75	0.86
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.57	0.86
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.09	0.86
1:A:22:LYS:HE3	1:A:24:TRP:HZ2	1.40	0.86
2:B:201:LYS:HZ3	2:B:204:GLU:HG2	1.41	0.86
2:B:149:LEU:HD21	2:B:159:ILE:HD12	1.56	0.85
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.59	0.85
1:A:494:ASN:ND2	2:B:289:LEU:HD12	1.93	0.84
1:A:454:LYS:HD2	1:A:552:VAL:CA	2.07	0.84
1:A:317:VAL:HG12	1:A:348:ASN:O	1.78	0.83
2:B:371:ALA:O	2:B:375:ILE:HG13	1.79	0.83
1:A:224:GLU:HB3	1:A:225:PRO:CD	2.09	0.83
2:B:257:ILE:O	2:B:261:VAL:HG23	1.79	0.83
1:A:53:GLU:C	1:A:55:PRO:HD3	1.99	0.82
2:B:216:THR:O	2:B:218:ASP:N	2.12	0.82
1:A:33:ALA:O	1:A:37:ILE:HG12	1.80	0.82
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:NE2	2:B:298:GLU:HB2	1.94	0.82
2:B:195:ILE:CD1	2:B:199:ARG:HE	1.92	0.81
2:B:244:ILE:HD13	2:B:244:ILE:H	1.43	0.81
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.63	0.81
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.46	0.81
2:B:362:THR:HG22	2:B:367:GLN:NE2	1.97	0.80
2:B:27:THR:O	2:B:31:ILE:HD12	1.81	0.80
2:B:278:GLN:HE22	2:B:298:GLU:HB2	1.44	0.79
1:A:238:LYS:HD3	1:A:315:HIS:ND1	1.97	0.79
2:B:277:ARG:HD3	2:B:277:ARG:H	1.48	0.79
1:A:288:ALA:HB1	1:A:291:GLU:CB	2.12	0.79
1:A:411:ILE:HD12	1:A:412:PRO:HD2	1.63	0.78
1:A:244:ILE:HD11	1:A:310:LEU:HD13	1.64	0.78
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.14	0.78
1:A:3:SER:HB2	1:A:5:ILE:HG13	1.66	0.77
2:B:366:LYS:O	2:B:370:GLU:HG3	1.84	0.77
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.67	0.76
1:A:104:LYS:HE2	1:A:104:LYS:N	1.99	0.76
2:B:215:THR:HB	2:B:217:PRO:HD3	1.66	0.76
2:B:310:LEU:HD23	2:B:310:LEU:O	1.86	0.76
2:B:249:LYS:HD2	2:B:252:TRP:CZ3	2.21	0.76
1:A:460:ASN:ND2	1:A:461:LYS:N	2.29	0.76
2:B:369:THR:HG22	2:B:373:GLN:NE2	2.00	0.76
1:A:506:ILE:HG21	1:A:533:LEU:CD1	2.16	0.76
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.16	0.76
2:B:369:THR:O	2:B:373:GLN:HG3	1.85	0.76
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.68	0.75
1:A:222:GLN:HG2	1:A:223:LYS:N	2.00	0.75
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.68	0.75
2:B:303:LEU:O	2:B:307:ARG:HB2	1.86	0.75
1:A:224:GLU:HB3	1:A:225:PRO:HD3	1.67	0.75
1:A:257:ILE:O	1:A:261:VAL:HG23	1.86	0.75
1:A:326:ILE:N	1:A:326:ILE:HD12	2.01	0.75
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.01	0.75
1:A:542:ILE:HG22	1:A:544:GLY:H	1.52	0.74
1:A:34:LEU:HB2	1:A:132:ILE:CD1	2.18	0.74
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.52	0.74
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.23	0.74
2:B:157:PRO:HG2	2:B:158:ALA:H	1.53	0.74
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.70	0.74
1:A:457:TYR:O	1:A:457:TYR:HD2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:HD3	2:B:72:ARG:HD2	1.70	0.73
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.24	0.73
1:A:438:GLU:HG3	1:A:460:ASN:HD21	1.54	0.73
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.69	0.73
1:A:506:ILE:HG21	1:A:533:LEU:HD12	1.71	0.73
1:A:3:SER:HB3	1:A:212:TRP:O	1.89	0.72
1:A:506:ILE:HD11	1:A:521:ILE:HG21	1.71	0.72
2:B:156:SER:N	2:B:157:PRO:HD2	2.04	0.72
1:A:106:VAL:HG12	1:A:107:THR:N	2.04	0.71
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.26	0.71
1:A:17:ASP:O	1:A:83:ARG:HD3	1.90	0.71
1:A:458:VAL:HG13	1:A:464:GLN:HG2	1.70	0.71
2:B:332:GLN:HB2	2:B:336:GLN:O	1.90	0.71
2:B:31:ILE:O	2:B:35:VAL:HG23	1.90	0.71
1:A:509:GLN:N	1:A:510:PRO:HD3	2.06	0.71
2:B:201:LYS:O	2:B:204:GLU:HB3	1.90	0.70
2:B:139:THR:HG22	2:B:140:PRO:CD	2.18	0.70
1:A:229:TRP:O	1:A:232:TYR:N	2.24	0.70
2:B:419:THR:H	2:B:420:PRO:HD2	1.56	0.70
1:A:470:THR:O	1:A:471:ASN:HB3	1.91	0.69
2:B:201:LYS:HZ2	2:B:204:GLU:HG2	1.58	0.69
1:A:328:GLU:HG2	1:A:390:LYS:CB	2.21	0.69
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.74	0.69
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.28	0.69
1:A:120:LEU:HB2	1:A:148:VAL:O	1.92	0.69
2:B:326:ILE:HB	2:B:342:TYR:CE1	2.27	0.68
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.28	0.68
1:A:510:PRO:O	1:A:522:ILE:HD13	1.92	0.68
2:B:359:GLY:O	2:B:361:HIS:N	2.24	0.68
1:A:297:GLU:HB2	1:A:298:GLU:OE2	1.93	0.68
1:A:215:THR:HG22	1:A:216:THR:N	2.08	0.68
1:A:34:LEU:HB2	1:A:132:ILE:HD11	1.76	0.68
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.08	0.68
1:A:224:GLU:CB	1:A:225:PRO:CD	2.72	0.67
1:A:179:VAL:HG22	1:A:190:GLY:O	1.95	0.67
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.22	0.67
2:B:364:ASP:O	2:B:367:GLN:N	2.28	0.67
2:B:366:LYS:HG3	2:B:405:TYR:CG	2.29	0.67
2:B:65:LYS:HZ1	2:B:409:THR:HG23	1.60	0.67
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.76	0.67
2:B:125:ARG:O	2:B:127:TYR:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HG	1:A:507:GLN:NE2	2.10	0.67
1:A:96:HIS:CD2	1:A:98:ALA:H	2.13	0.67
2:B:263:LYS:HE3	2:B:425:LEU:CB	2.25	0.67
2:B:282:LEU:HG	2:B:293:ILE:HD12	1.78	0.66
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.28	0.66
2:B:298:GLU:HB3	2:B:301:LEU:HD13	1.78	0.66
2:B:303:LEU:O	2:B:307:ARG:HD2	1.94	0.66
2:B:422:LEU:HA	2:B:425:LEU:HD12	1.76	0.66
1:A:328:GLU:CG	1:A:390:LYS:HB2	2.25	0.66
1:A:410:TRP:HB2	2:B:365:VAL:HG21	1.78	0.66
2:B:86:ASP:O	2:B:89:GLU:HG2	1.95	0.66
2:B:32:LYS:O	2:B:36:GLU:HG2	1.96	0.66
1:A:540:LYS:CD	2:B:265:ASN:HD21	2.03	0.66
1:A:544:GLY:O	1:A:548:VAL:HG23	1.96	0.65
1:A:288:ALA:CB	1:A:291:GLU:HB3	2.24	0.65
1:A:498:ASP:HB2	1:A:538:ALA:HA	1.77	0.65
1:A:23:GLN:HG2	1:A:25:PRO:HD2	1.79	0.65
1:A:393:ILE:HG23	1:A:414:TRP:CZ3	2.31	0.65
1:A:402:TRP:HE3	1:A:402:TRP:O	1.79	0.65
2:B:224:GLU:O	2:B:226:PRO:HD3	1.96	0.65
2:B:245:VAL:HG12	2:B:246:LEU:N	2.11	0.65
2:B:246:LEU:HD21	2:B:310:LEU:HD13	1.77	0.65
2:B:268:SER:HA	2:B:271:TYR:O	1.96	0.65
2:B:339:TYR:C	2:B:340:GLN:OE1	2.34	0.65
1:A:1:PRO:O	1:A:117:SER:HA	1.95	0.65
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.79	0.65
1:A:115:TYR:CE2	1:A:151:GLN:HA	2.32	0.64
2:B:175:ASN:OD1	2:B:201:LYS:HE3	1.98	0.64
2:B:345:PRO:HB2	2:B:346:PHE:CE1	2.33	0.64
1:A:124:PHE:O	1:A:124:PHE:CD2	2.51	0.64
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.27	0.64
1:A:540:LYS:O	1:A:540:LYS:HG3	1.96	0.64
1:A:278:GLN:HG2	1:A:302:GLU:OE2	1.97	0.64
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.33	0.64
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.32	0.64
1:A:514:GLU:O	1:A:516:GLU:N	2.29	0.64
2:B:178:ILE:HG22	2:B:191:SER:HB3	1.78	0.64
2:B:246:LEU:HD21	2:B:310:LEU:CD1	2.28	0.64
1:A:399:GLU:HG3	1:A:402:TRP:HE1	1.61	0.64
2:B:171:PHE:HE1	2:B:178:ILE:HD11	1.63	0.64
2:B:278:GLN:OE1	2:B:297:GLU:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:GLY:O	2:B:355:ALA:HA	1.98	0.64
1:A:495:ILE:HB	1:A:533:LEU:HD23	1.81	0.63
1:A:458:VAL:HG13	1:A:464:GLN:CG	2.28	0.63
2:B:22:LYS:CE	2:B:22:LYS:HA	2.16	0.63
1:A:304:ALA:O	1:A:307:ARG:HB2	1.99	0.63
1:A:131:THR:HG1	1:A:143:ARG:HE	1.46	0.63
1:A:173:LYS:O	1:A:176:PRO:HD3	1.98	0.63
1:A:34:LEU:CB	1:A:132:ILE:HD12	2.28	0.63
1:A:85:GLN:HE22	2:B:53:GLU:HB2	1.62	0.63
2:B:161:GLN:O	2:B:162:SER:C	2.37	0.63
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.34	0.63
2:B:282:LEU:HG	2:B:293:ILE:CD1	2.29	0.63
2:B:149:LEU:HD13	2:B:156:SER:HA	1.80	0.63
2:B:372:VAL:HG12	2:B:373:GLN:N	2.13	0.63
1:A:108:VAL:HG13	1:A:227:PHE:CE1	2.33	0.63
1:A:548:VAL:O	1:A:551:LEU:HB2	1.99	0.63
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.81	0.62
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.80	0.62
1:A:506:ILE:HG22	1:A:507:GLN:N	2.14	0.62
1:A:417:VAL:O	1:A:417:VAL:HG12	1.98	0.62
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.35	0.62
1:A:10:VAL:HG12	1:A:11:LYS:N	2.14	0.62
2:B:171:PHE:O	2:B:175:ASN:HB2	2.00	0.62
2:B:206:ARG:HG2	2:B:206:ARG:HH11	1.65	0.62
2:B:418:ASN:O	2:B:419:THR:HG23	1.99	0.62
2:B:65:LYS:NZ	2:B:409:THR:HG23	2.15	0.62
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.82	0.62
1:A:282:LEU:O	1:A:284:ARG:N	2.33	0.61
2:B:255:ASN:OD1	2:B:259:LYS:HE3	2.00	0.61
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.82	0.61
1:A:164:MET:CE	1:A:187:LEU:HD13	2.30	0.61
1:A:155:GLY:O	1:A:159:ILE:HG13	2.00	0.61
1:A:465:LYS:HG3	1:A:466:VAL:N	2.15	0.61
2:B:246:LEU:N	2:B:246:LEU:HD23	2.16	0.61
1:A:3:SER:CB	1:A:5:ILE:HG13	2.31	0.61
1:A:138:GLU:OE1	1:A:138:GLU:O	2.19	0.61
2:B:253:THR:HA	2:B:292:VAL:HA	1.82	0.61
1:A:335:GLY:HA2	1:A:367:GLN:NE2	2.14	0.61
1:A:457:TYR:HD2	1:A:457:TYR:C	2.04	0.61
2:B:171:PHE:CE1	2:B:178:ILE:HD11	2.35	0.61
1:A:497:THR:CG2	1:A:499:SER:HB3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLU:H	1:A:55:PRO:CD	2.13	0.60
2:B:402:TRP:O	2:B:406:TRP:HB2	2.02	0.60
2:B:253:THR:O	2:B:257:ILE:HG22	2.00	0.60
1:A:21:VAL:HG22	1:A:58:THR:HA	1.83	0.60
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.31	0.60
1:A:54:ASN:N	1:A:55:PRO:HD3	2.17	0.60
1:A:75:VAL:HG12	1:A:76:ASP:N	2.17	0.60
1:A:65:LYS:HG2	1:A:68:SER:HB3	1.83	0.60
1:A:344:GLU:HA	1:A:344:GLU:OE1	2.02	0.60
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.84	0.59
2:B:241:VAL:HG12	2:B:243:PRO:CD	2.29	0.59
1:A:241:VAL:HG12	1:A:242:GLN:N	2.16	0.59
2:B:91:GLN:O	2:B:92:LEU:HD23	2.01	0.59
2:B:215:THR:CB	2:B:217:PRO:HD3	2.32	0.59
1:A:10:VAL:HG12	1:A:11:LYS:H	1.67	0.59
1:A:220:LYS:HE3	1:A:221:HIS:CD2	2.37	0.59
1:A:34:LEU:HB2	1:A:132:ILE:HD12	1.84	0.59
1:A:188:TYR:CD2	3:A:701:TPB:H411	2.37	0.59
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.37	0.59
1:A:194:GLU:O	1:A:196:GLY:N	2.35	0.59
1:A:536:VAL:HG11	1:A:542:ILE:CD1	2.32	0.59
1:A:540:LYS:HD2	2:B:265:ASN:ND2	2.08	0.59
1:A:101:LYS:HD2	1:A:101:LYS:H	1.67	0.59
1:A:206:ARG:HH21	1:A:217:PRO:C	2.06	0.59
1:A:22:LYS:HG2	1:A:24:TRP:CZ2	2.38	0.59
1:A:106:VAL:CG1	1:A:107:THR:H	2.13	0.58
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.85	0.58
1:A:56:TYR:N	1:A:56:TYR:CD1	2.70	0.58
2:B:220:LYS:NZ	2:B:231:GLY:HA3	2.18	0.58
1:A:55:PRO:HB2	1:A:143:ARG:NH2	2.19	0.58
2:B:18:GLY:HA3	2:B:127:TYR:CE1	2.37	0.58
1:A:35:VAL:O	1:A:39:THR:HG23	2.04	0.58
1:A:441:TYR:HB2	1:A:458:VAL:O	2.03	0.58
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.68	0.58
2:B:104:LYS:HA	2:B:237:ASP:OD2	2.03	0.58
2:B:362:THR:HG23	2:B:366:LYS:HZ3	1.69	0.58
1:A:34:LEU:HD12	1:A:132:ILE:HG13	1.85	0.58
1:A:468:PRO:O	1:A:469:LEU:HD23	2.03	0.58
2:B:163:SER:O	2:B:167:ILE:HG13	2.04	0.58
1:A:131:THR:OG1	1:A:143:ARG:NE	2.36	0.58
1:A:315:HIS:CE1	1:A:347:LYS:HD3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASN:HA	2:B:309:ILE:HG22	1.85	0.58
1:A:96:HIS:HD2	1:A:97:PRO:N	2.02	0.57
2:B:364:ASP:O	2:B:367:GLN:HB2	2.03	0.57
1:A:246:LEU:HD13	1:A:303:LEU:HD11	1.86	0.57
1:A:270:ILE:HG13	1:A:314:VAL:HG12	1.84	0.57
2:B:125:ARG:O	2:B:126:LYS:C	2.41	0.57
1:A:335:GLY:O	1:A:355:ALA:HA	2.04	0.57
2:B:278:GLN:HE22	2:B:298:GLU:CB	2.17	0.57
2:B:342:TYR:C	2:B:342:TYR:CD1	2.77	0.57
1:A:373:GLN:HG2	2:B:394:GLN:HE22	1.69	0.57
2:B:206:ARG:HG2	2:B:206:ARG:NH1	2.19	0.57
1:A:399:GLU:HG3	1:A:402:TRP:NE1	2.19	0.57
1:A:62:ALA:HB1	1:A:71:TRP:HD1	1.70	0.57
2:B:115:TYR:O	2:B:117:SER:N	2.38	0.57
2:B:330:GLN:HG2	2:B:338:THR:HG1	1.70	0.57
1:A:306:ASN:O	1:A:310:LEU:HG	2.04	0.57
1:A:19:PRO:O	1:A:56:TYR:HB3	2.05	0.57
1:A:33:ALA:O	1:A:36:GLU:HB2	2.04	0.57
1:A:457:TYR:CD2	1:A:457:TYR:C	2.77	0.57
1:A:476:LYS:HD3	1:A:517:LEU:HD22	1.87	0.57
1:A:398:TRP:CZ2	1:A:411:ILE:HB	2.40	0.57
2:B:173:LYS:O	2:B:176:PRO:HD3	2.05	0.57
1:A:454:LYS:CG	1:A:552:VAL:HA	2.35	0.56
1:A:368:LEU:O	1:A:372:VAL:HG23	2.06	0.56
1:A:101:LYS:N	1:A:101:LYS:HD2	2.20	0.56
1:A:276:VAL:HG12	1:A:276:VAL:O	2.04	0.56
2:B:155:GLY:O	2:B:159:ILE:HG13	2.04	0.56
1:A:254:VAL:HG21	1:A:288:ALA:HB3	1.86	0.56
2:B:419:THR:N	2:B:420:PRO:HD2	2.21	0.56
1:A:372:VAL:HG11	1:A:411:ILE:CD1	2.36	0.56
1:A:518:VAL:O	1:A:522:ILE:HG13	2.05	0.56
2:B:161:GLN:O	2:B:164:MET:N	2.39	0.56
2:B:293:ILE:HB	2:B:294:PRO:HD2	1.88	0.56
1:A:506:ILE:HG21	1:A:533:LEU:HD11	1.88	0.56
2:B:13:LYS:O	2:B:16:MET:HB2	2.06	0.56
2:B:175:ASN:N	2:B:176:PRO:CD	2.69	0.56
1:A:315:HIS:HE2	1:A:347:LYS:HD3	1.69	0.56
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.87	0.56
1:A:164:MET:HE2	1:A:187:LEU:HD13	1.87	0.56
2:B:120:LEU:HD13	2:B:149:LEU:HD23	1.88	0.56
2:B:115:TYR:OH	2:B:184:MET:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TRP:NE1	1:A:411:ILE:HG21	2.21	0.55
2:B:244:ILE:CD1	2:B:244:ILE:H	2.16	0.55
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.94	0.55
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.41	0.55
2:B:278:GLN:O	2:B:281:LYS:HG2	2.06	0.55
1:A:178:ILE:HD11	1:A:201:LYS:HG2	1.89	0.55
1:A:241:VAL:CG1	1:A:242:GLN:N	2.69	0.55
2:B:298:GLU:HB3	2:B:301:LEU:HB3	1.88	0.55
1:A:244:ILE:HD11	1:A:310:LEU:HD22	1.88	0.55
1:A:353:LYS:O	1:A:374:LYS:NZ	2.38	0.55
1:A:53:GLU:N	1:A:55:PRO:HD3	2.16	0.55
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.89	0.55
1:A:317:VAL:O	1:A:349:LEU:HD12	2.07	0.55
1:A:457:TYR:O	1:A:457:TYR:CD2	2.58	0.55
1:A:542:ILE:HG22	1:A:543:GLY:N	2.21	0.55
1:A:92:LEU:HD13	2:B:22:LYS:HD2	1.88	0.55
2:B:67:ASP:O	2:B:68:SER:O	2.25	0.55
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.42	0.55
2:B:244:ILE:HD13	2:B:244:ILE:N	2.19	0.55
1:A:202:ILE:O	1:A:205:LEU:HB3	2.07	0.54
2:B:193:LEU:O	2:B:194:GLU:C	2.44	0.54
1:A:497:THR:HG22	1:A:498:ASP:N	2.21	0.54
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.90	0.54
2:B:296:THR:HG22	2:B:297:GLU:N	2.22	0.54
1:A:479:LEU:O	1:A:521:ILE:HD11	2.08	0.54
2:B:160:PHE:O	2:B:161:GLN:C	2.46	0.54
1:A:543:GLY:CA	2:B:284:ARG:HH11	2.16	0.54
2:B:56:TYR:HE2	2:B:126:LYS:HD2	1.73	0.54
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.43	0.54
1:A:543:GLY:HA3	2:B:284:ARG:NH1	2.16	0.54
1:A:58:THR:HG22	1:A:59:PRO:CD	2.37	0.54
2:B:330:GLN:NE2	2:B:338:THR:O	2.37	0.54
1:A:402:TRP:CE3	1:A:402:TRP:O	2.60	0.54
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.43	0.54
2:B:296:THR:O	2:B:297:GLU:C	2.46	0.54
1:A:84:THR:HG21	1:A:153:TRP:NE1	2.16	0.54
1:A:128:THR:CB	1:A:146:TYR:HB2	2.38	0.53
1:A:362:THR:HG23	1:A:366:LYS:HD3	1.90	0.53
1:A:547:GLN:O	1:A:551:LEU:HG	2.08	0.53
2:B:168:LEU:C	2:B:170:PRO:HD2	2.29	0.53
2:B:278:GLN:HA	2:B:281:LYS:CE	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASN:O	2:B:308:GLU:N	2.41	0.53
2:B:388:LYS:HG3	2:B:413:GLU:HB2	1.89	0.53
1:A:290:THR:O	1:A:290:THR:HG22	2.08	0.53
2:B:342:TYR:C	2:B:342:TYR:HD1	2.12	0.53
1:A:220:LYS:HE3	1:A:221:HIS:NE2	2.23	0.53
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.43	0.53
1:A:309:ILE:HG22	1:A:310:LEU:N	2.24	0.53
1:A:111:VAL:O	1:A:114:ALA:HB3	2.08	0.53
2:B:104:LYS:HB2	2:B:192:ASP:OD1	2.09	0.53
2:B:198:HIS:O	2:B:200:THR:N	2.42	0.53
1:A:112:GLY:HA2	1:A:185:ASP:OD1	2.09	0.53
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.91	0.53
1:A:10:VAL:CG1	1:A:11:LYS:H	2.21	0.52
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.89	0.52
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.87	0.52
2:B:200:THR:O	2:B:201:LYS:C	2.48	0.52
2:B:207:GLN:O	2:B:208:HIS:C	2.48	0.52
2:B:362:THR:HG23	2:B:366:LYS:NZ	2.25	0.52
2:B:277:ARG:H	2:B:277:ARG:CD	2.21	0.52
1:A:104:LYS:HG2	1:A:192:ASP:HA	1.92	0.52
1:A:215:THR:HG22	1:A:216:THR:H	1.73	0.52
1:A:497:THR:HG22	1:A:499:SER:HB3	1.91	0.52
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.45	0.52
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.92	0.52
1:A:73:LYS:NZ	1:A:130:PHE:CZ	2.74	0.52
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.91	0.52
1:A:376:THR:O	1:A:380:ILE:HG13	2.10	0.52
1:A:411:ILE:HG23	1:A:411:ILE:O	2.10	0.52
1:A:215:THR:CG2	1:A:216:THR:N	2.73	0.51
1:A:509:GLN:H	1:A:510:PRO:HD3	1.74	0.51
2:B:215:THR:C	2:B:217:PRO:HD3	2.30	0.51
2:B:2:ILE:O	2:B:4:PRO:CD	2.53	0.51
1:A:77:PHE:O	1:A:80:LEU:N	2.29	0.51
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.45	0.51
2:B:228:LEU:C	2:B:230:MET:H	2.11	0.51
2:B:31:ILE:HG22	2:B:35:VAL:CG2	2.41	0.51
1:A:31:ILE:HG21	1:A:134:SER:O	2.11	0.51
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.26	0.51
1:A:244:ILE:HD11	1:A:310:LEU:CD1	2.36	0.51
1:A:350:LYS:HG2	1:A:351:THR:N	2.25	0.51
1:A:35:VAL:HG12	1:A:35:VAL:O	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:PRO:HB2	1:A:522:ILE:HD11	1.92	0.51
2:B:210:LEU:O	2:B:210:LEU:HD12	2.10	0.51
2:B:421:PRO:HG2	2:B:422:LEU:H	1.74	0.51
1:A:102:LYS:O	1:A:103:LYS:HD3	2.10	0.51
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.76	0.51
1:A:3:SER:OG	1:A:5:ILE:CD1	2.58	0.51
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.11	0.51
2:B:94:ILE:HG12	2:B:161:GLN:CD	2.31	0.51
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.43	0.51
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.43	0.51
2:B:157:PRO:HG2	2:B:158:ALA:N	2.25	0.51
2:B:226:PRO:O	2:B:228:LEU:N	2.44	0.51
1:A:173:LYS:C	1:A:175:ASN:H	2.14	0.51
1:A:301:LEU:HD12	1:A:301:LEU:O	2.10	0.51
1:A:13:LYS:HB2	1:A:16:MET:HG3	1.93	0.51
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.75	0.51
1:A:308:GLU:O	1:A:311:LYS:HG2	2.11	0.50
2:B:377:THR:O	2:B:378:GLU:C	2.48	0.50
2:B:245:VAL:CG1	2:B:246:LEU:N	2.73	0.50
2:B:385:LYS:O	2:B:385:LYS:HG3	2.10	0.50
2:B:301:LEU:O	2:B:301:LEU:HD23	2.10	0.50
1:A:224:GLU:O	1:A:226:PRO:O	2.29	0.50
1:A:30:LYS:O	1:A:32:LYS:N	2.45	0.50
1:A:390:LYS:O	1:A:391:LEU:HD23	2.10	0.50
1:A:81:ASN:C	1:A:83:ARG:H	2.15	0.50
1:A:91:GLN:HE21	1:A:184:MET:CE	2.24	0.50
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.46	0.50
2:B:215:THR:C	2:B:217:PRO:CD	2.80	0.50
2:B:296:THR:HB	2:B:299:ALA:HB2	1.93	0.50
1:A:435:VAL:CG1	2:B:290:THR:HG21	2.39	0.50
1:A:21:VAL:CG2	1:A:58:THR:HA	2.42	0.50
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.97	0.50
1:A:511:ASP:OD1	1:A:512:LYS:HG2	2.12	0.50
1:A:62:ALA:HB1	1:A:71:TRP:CD1	2.45	0.50
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.94	0.50
1:A:10:VAL:CG1	1:A:11:LYS:N	2.75	0.49
1:A:208:HIS:HA	1:A:211:ARG:NH1	2.27	0.49
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.47	0.49
1:A:84:THR:HG22	1:A:124:PHE:CZ	2.46	0.49
2:B:257:ILE:HD12	2:B:282:LEU:HD23	1.94	0.49
1:A:12:LEU:O	1:A:13:LYS:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLU:N	1:A:449:GLU:CD	2.66	0.49
2:B:174:GLN:O	2:B:175:ASN:CG	2.51	0.49
1:A:382:ILE:HG23	2:B:136:ASN:ND2	2.26	0.49
1:A:75:VAL:HG12	1:A:76:ASP:H	1.76	0.49
1:A:100:LEU:HD22	3:A:701:TPB:N1	2.27	0.49
1:A:246:LEU:HD13	1:A:303:LEU:CD1	2.41	0.49
1:A:311:LYS:HE3	1:A:312:GLU:OE2	2.12	0.49
2:B:201:LYS:HZ3	2:B:204:GLU:CG	2.19	0.49
2:B:56:TYR:CE2	2:B:126:LYS:HD2	2.47	0.49
1:A:536:VAL:HG11	1:A:542:ILE:HG13	1.95	0.49
1:A:102:LYS:HA	1:A:318:TYR:HD1	1.76	0.49
1:A:330:GLN:NE2	1:A:340:GLN:HE22	1.98	0.49
1:A:440:PHE:CE1	1:A:489:SER:CB	2.96	0.49
1:A:59:PRO:O	1:A:75:VAL:HG13	2.13	0.49
1:A:132:ILE:O	1:A:132:ILE:HG23	2.12	0.49
2:B:327:ALA:HA	2:B:340:GLN:O	2.12	0.49
1:A:513:SER:O	1:A:519:ASN:ND2	2.46	0.48
2:B:278:GLN:HA	2:B:281:LYS:HG2	1.94	0.48
1:A:410:TRP:HB2	2:B:365:VAL:CG2	2.42	0.48
2:B:54:ASN:HD21	2:B:126:LYS:HA	1.78	0.48
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.31	0.48
1:A:301:LEU:O	1:A:305:GLU:HG3	2.13	0.48
1:A:449:GLU:N	1:A:449:GLU:OE1	2.46	0.48
3:A:701:TPB:H16	3:A:701:TPB:N1	2.27	0.48
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.24	0.48
2:B:337:TRP:CD1	2:B:337:TRP:N	2.81	0.48
1:A:131:THR:OG1	1:A:143:ARG:CD	2.61	0.48
1:A:210:LEU:HD12	1:A:210:LEU:O	2.14	0.48
1:A:497:THR:HG22	1:A:499:SER:N	2.28	0.48
1:A:503:LEU:HD22	1:A:535:TRP:CB	2.36	0.48
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.48	0.48
2:B:418:ASN:O	2:B:419:THR:CG2	2.62	0.48
1:A:293:ILE:HG23	1:A:294:PRO:HD2	1.96	0.48
1:A:38:CYS:HB3	1:A:144:TYR:CZ	2.49	0.48
1:A:394:GLN:O	1:A:395:LYS:C	2.51	0.48
2:B:216:THR:N	2:B:217:PRO:CD	2.76	0.48
2:B:305:GLU:O	2:B:308:GLU:HB3	2.14	0.48
1:A:282:LEU:C	1:A:284:ARG:H	2.17	0.48
2:B:115:TYR:CD2	2:B:115:TYR:N	2.78	0.48
2:B:193:LEU:HD12	2:B:198:HIS:N	2.29	0.48
2:B:279:LEU:O	2:B:282:LEU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLN:NE2	1:A:395:LYS:H	2.11	0.48
2:B:149:LEU:HD13	2:B:156:SER:CA	2.44	0.48
1:A:100:LEU:HD22	3:A:701:TPB:C9	2.44	0.48
1:A:242:GLN:HE21	1:A:244:ILE:HG22	1.79	0.48
1:A:54:ASN:N	1:A:55:PRO:CD	2.76	0.48
1:A:77:PHE:CZ	1:A:150:PRO:HB3	2.49	0.48
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.49	0.48
1:A:442:VAL:HG13	1:A:481:ALA:CB	2.42	0.48
1:A:98:ALA:HB1	1:A:350:LYS:HB2	1.96	0.48
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.43	0.47
1:A:493:VAL:HG22	1:A:494:ASN:N	2.29	0.47
1:A:103:LYS:C	1:A:104:LYS:HE2	2.33	0.47
1:A:108:VAL:CG1	1:A:227:PHE:CE1	2.97	0.47
1:A:506:ILE:CG2	1:A:507:GLN:N	2.77	0.47
1:A:326:ILE:CD1	1:A:326:ILE:N	2.71	0.47
1:A:255:ASN:HD22	1:A:289:LEU:HD11	1.78	0.47
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.50	0.47
1:A:470:THR:O	1:A:471:ASN:CB	2.57	0.47
2:B:195:ILE:CG1	2:B:199:ARG:HG3	2.45	0.47
2:B:394:GLN:HE21	2:B:396:GLU:HB2	1.79	0.47
1:A:395:LYS:O	1:A:396:GLU:C	2.53	0.47
1:A:66:LYS:C	1:A:68:SER:H	2.18	0.47
2:B:276:VAL:O	2:B:279:LEU:N	2.42	0.47
2:B:297:GLU:HG2	2:B:298:GLU:HG2	1.96	0.47
1:A:178:ILE:HD11	1:A:201:LYS:CG	2.45	0.47
1:A:65:LYS:HG2	1:A:68:SER:CA	2.45	0.47
2:B:416:PHE:N	2:B:416:PHE:CD2	2.82	0.47
1:A:483:TYR:HB2	1:A:521:ILE:CG1	2.45	0.47
2:B:320:ASP:O	2:B:343:GLN:NE2	2.33	0.47
2:B:266:TRP:HB2	2:B:422:LEU:HD23	1.97	0.47
1:A:18:GLY:CA	1:A:56:TYR:CD2	2.98	0.47
2:B:375:ILE:O	2:B:376:THR:C	2.53	0.47
1:A:19:PRO:O	1:A:56:TYR:CB	2.63	0.47
1:A:242:GLN:O	1:A:242:GLN:HG3	2.14	0.47
1:A:397:THR:O	1:A:400:THR:HB	2.14	0.47
2:B:85:GLN:O	2:B:85:GLN:HG2	2.13	0.47
1:A:30:LYS:O	1:A:33:ALA:N	2.48	0.47
2:B:156:SER:N	2:B:157:PRO:CD	2.76	0.47
1:A:92:LEU:CD1	2:B:22:LYS:HD2	2.44	0.47
1:A:229:TRP:O	1:A:231:GLY:N	2.48	0.47
1:A:288:ALA:HB2	1:A:291:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:N	1:A:298:GLU:CD	2.51	0.47
1:A:362:THR:HG22	1:A:363:ASN:N	2.30	0.47
1:A:507:GLN:O	1:A:509:GLN:HG3	2.14	0.47
2:B:152:GLY:O	2:B:184:MET:HE3	2.15	0.46
2:B:200:THR:C	2:B:202:ILE:N	2.65	0.46
2:B:323:LYS:NZ	2:B:344:GLU:OE1	2.27	0.46
2:B:388:LYS:HE2	2:B:415:GLU:OE1	2.15	0.46
2:B:65:LYS:NZ	2:B:409:THR:CG2	2.78	0.46
2:B:85:GLN:CG	2:B:85:GLN:O	2.62	0.46
2:B:306:ASN:C	2:B:308:GLU:N	2.69	0.46
1:A:115:TYR:O	1:A:149:LEU:HB2	2.15	0.46
1:A:77:PHE:CE1	1:A:150:PRO:HB3	2.50	0.46
1:A:509:GLN:N	1:A:510:PRO:CD	2.78	0.46
2:B:330:GLN:HE21	2:B:338:THR:C	2.19	0.46
1:A:120:LEU:HD23	1:A:125:ARG:CG	2.45	0.46
1:A:277:ARG:NH2	1:A:514:GLU:OE1	2.44	0.46
2:B:254:VAL:O	2:B:258:GLN:HG3	2.15	0.46
2:B:296:THR:CG2	2:B:297:GLU:N	2.79	0.46
1:A:483:TYR:O	1:A:487:GLN:HG3	2.16	0.46
2:B:146:TYR:CD1	2:B:150:PRO:HB3	2.50	0.46
1:A:225:PRO:HA	1:A:226:PRO:C	2.36	0.46
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.81	0.46
2:B:309:ILE:HG13	2:B:312:GLU:OE2	2.15	0.46
1:A:182:GLN:HG3	1:A:182:GLN:O	2.15	0.46
1:A:397:THR:HG21	1:A:424:LYS:HA	1.98	0.46
1:A:19:PRO:HG2	1:A:80:LEU:HA	1.97	0.46
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.51	0.46
2:B:300:GLU:HA	2:B:300:GLU:OE1	2.15	0.46
2:B:305:GLU:HG3	2:B:306:ASN:N	2.31	0.46
2:B:198:HIS:C	2:B:200:THR:N	2.68	0.45
2:B:266:TRP:CG	2:B:422:LEU:HD23	2.51	0.45
2:B:191:SER:OG	2:B:198:HIS:ND1	2.36	0.45
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.16	0.45
1:A:513:SER:O	1:A:519:ASN:OD1	2.34	0.45
1:A:82:LYS:HG2	1:A:82:LYS:O	2.17	0.45
1:A:3:SER:C	1:A:5:ILE:H	2.20	0.45
1:A:477:THR:C	1:A:479:LEU:H	2.20	0.45
1:A:96:HIS:CD2	1:A:97:PRO:N	2.83	0.45
2:B:238:LYS:O	2:B:240:THR:N	2.49	0.45
2:B:34:LEU:O	2:B:35:VAL:C	2.54	0.45
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.32	0.45
1:A:38:CYS:SG	1:A:144:TYR:CE2	3.10	0.45
2:B:183:TYR:O	2:B:184:MET:HB2	2.16	0.45
1:A:24:TRP:N	1:A:24:TRP:CD1	2.84	0.45
1:A:376:THR:HG23	1:A:386:THR:HG22	1.97	0.45
1:A:500:GLN:H	1:A:500:GLN:HG3	1.49	0.45
1:A:96:HIS:CE1	1:A:350:LYS:HE2	2.51	0.45
2:B:223:LYS:C	2:B:225:PRO:HD3	2.37	0.45
2:B:364:ASP:O	2:B:365:VAL:C	2.55	0.45
2:B:84:THR:O	2:B:86:ASP:N	2.49	0.45
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.17	0.45
1:A:438:GLU:HG3	1:A:460:ASN:ND2	2.27	0.45
2:B:58:THR:HA	2:B:59:PRO:HD3	1.81	0.45
1:A:22:LYS:HE3	1:A:24:TRP:CZ2	2.33	0.45
1:A:282:LEU:C	1:A:284:ARG:N	2.70	0.45
1:A:32:LYS:O	1:A:36:GLU:HG3	2.17	0.45
1:A:115:TYR:OH	1:A:151:GLN:HB2	2.17	0.45
1:A:356:ARG:NH1	1:A:358:ARG:HD2	2.32	0.45
2:B:179:VAL:HG23	2:B:179:VAL:O	2.15	0.45
1:A:379:SER:HA	1:A:383:TRP:CE3	2.52	0.45
1:A:477:THR:C	1:A:479:LEU:N	2.71	0.44
2:B:115:TYR:C	2:B:117:SER:H	2.18	0.44
2:B:301:LEU:O	2:B:305:GLU:HB3	2.17	0.44
1:A:115:TYR:OH	1:A:151:GLN:CB	2.65	0.44
1:A:13:LYS:HD2	1:A:16:MET:CE	2.47	0.44
1:A:215:THR:CG2	1:A:216:THR:H	2.30	0.44
1:A:174:GLN:O	1:A:175:ASN:CG	2.56	0.44
1:A:22:LYS:HB3	1:A:24:TRP:NE1	2.32	0.44
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.53	0.44
2:B:280:SER:O	2:B:283:LEU:N	2.46	0.44
1:A:151:GLN:O	1:A:151:GLN:HG3	2.17	0.44
1:A:167:ILE:O	1:A:170:PRO:HD2	2.17	0.44
1:A:206:ARG:HH21	1:A:217:PRO:CA	2.31	0.44
1:A:242:GLN:HG2	1:A:266:TRP:HE1	1.81	0.44
2:B:314:VAL:HG13	2:B:317:VAL:HG21	1.98	0.44
1:A:128:THR:HB	1:A:146:TYR:HB2	2.00	0.44
1:A:183:TYR:CE2	1:A:230:MET:SD	3.11	0.44
1:A:3:SER:HB3	1:A:212:TRP:C	2.37	0.44
2:B:278:GLN:C	2:B:281:LYS:HG2	2.36	0.44
1:A:373:GLN:HG2	2:B:394:GLN:NE2	2.30	0.44
1:A:108:VAL:HG13	1:A:227:PHE:HE1	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG12	1:A:51:GLY:N	2.33	0.44
1:A:543:GLY:CA	2:B:284:ARG:NH1	2.78	0.44
2:B:6:GLU:O	2:B:7:THR:O	2.35	0.44
1:A:57:ASN:HA	1:A:129:ALA:O	2.17	0.44
1:A:382:ILE:HA	2:B:136:ASN:HD22	1.83	0.44
1:A:483:TYR:CE2	1:A:487:GLN:NE2	2.86	0.44
2:B:226:PRO:O	2:B:227:PHE:C	2.56	0.44
2:B:245:VAL:CG1	2:B:246:LEU:H	2.31	0.44
1:A:35:VAL:CG1	1:A:35:VAL:O	2.65	0.44
1:A:55:PRO:HB2	1:A:143:ARG:HH22	1.82	0.44
1:A:259:LYS:HG2	1:A:263:LYS:HE3	2.00	0.44
1:A:328:GLU:HA	1:A:390:LYS:O	2.17	0.44
1:A:438:GLU:OE2	1:A:461:LYS:HB2	2.17	0.44
2:B:229:TRP:N	2:B:229:TRP:CD1	2.85	0.44
2:B:363:ASN:O	2:B:367:GLN:NE2	2.51	0.44
2:B:232:TYR:CE1	2:B:234:LEU:HD21	2.53	0.43
1:A:254:VAL:O	1:A:258:GLN:HG3	2.18	0.43
2:B:298:GLU:O	2:B:302:GLU:N	2.51	0.43
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.45	0.43
1:A:536:VAL:HG11	1:A:542:ILE:HD12	2.01	0.43
1:A:65:LYS:HG2	1:A:68:SER:CB	2.47	0.43
1:A:77:PHE:CD2	1:A:80:LEU:CD2	3.01	0.43
2:B:216:THR:HG22	2:B:216:THR:O	2.17	0.43
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.48	0.43
1:A:442:VAL:CG1	1:A:443:ASP:N	2.80	0.43
1:A:492:GLU:CD	1:A:530:LYS:HD2	2.38	0.43
1:A:84:THR:CG2	1:A:124:PHE:HZ	2.31	0.43
1:A:324:ASP:O	1:A:343:GLN:HG2	2.19	0.43
1:A:9:PRO:O	1:A:9:PRO:HG2	2.18	0.43
2:B:178:ILE:HG22	2:B:191:SER:CB	2.48	0.43
2:B:72:ARG:HH11	2:B:72:ARG:HG3	1.82	0.43
1:A:111:VAL:O	1:A:114:ALA:CB	2.66	0.43
1:A:476:LYS:HD3	1:A:517:LEU:CD2	2.49	0.43
1:A:361:HIS:HD2	1:A:513:SER:HB2	1.84	0.43
1:A:17:ASP:OD2	1:A:56:TYR:HE2	2.02	0.43
2:B:84:THR:HG21	2:B:124:PHE:CZ	2.53	0.43
2:B:136:ASN:O	2:B:137:ASN:C	2.56	0.43
1:A:447:ASN:ND2	1:A:450:THR:HG23	2.34	0.43
1:A:54:ASN:O	1:A:55:PRO:C	2.57	0.43
1:A:5:ILE:HG22	1:A:6:GLU:O	2.18	0.43
2:B:249:LYS:HD2	2:B:252:TRP:HZ3	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:O	1:A:199:ARG:HG3	2.18	0.43
2:B:27:THR:HG22	2:B:29:GLU:H	1.84	0.43
1:A:27:THR:O	1:A:28:GLU:C	2.56	0.43
1:A:30:LYS:HD3	1:A:62:ALA:HB3	2.01	0.43
1:A:341:ILE:O	1:A:349:LEU:HB3	2.19	0.43
1:A:363:ASN:OD1	1:A:364:ASP:N	2.51	0.42
1:A:397:THR:HB	1:A:398:TRP:H	1.66	0.42
1:A:400:THR:O	1:A:403:THR:HB	2.19	0.42
1:A:483:TYR:CE2	1:A:487:GLN:CD	2.92	0.42
1:A:497:THR:HG21	1:A:499:SER:HB3	2.00	0.42
1:A:91:GLN:O	1:A:92:LEU:C	2.56	0.42
2:B:12:LEU:HD11	2:B:127:TYR:CE2	2.54	0.42
2:B:53:GLU:OE1	2:B:53:GLU:N	2.44	0.42
1:A:121:ASP:O	1:A:122:GLU:C	2.56	0.42
2:B:104:LYS:HB3	2:B:192:ASP:HA	2.00	0.42
1:A:183:TYR:OH	1:A:230:MET:SD	2.74	0.42
2:B:11:LYS:NZ	2:B:14:PRO:HG3	2.34	0.42
2:B:362:THR:HG22	2:B:363:ASN:O	2.19	0.42
1:A:317:VAL:HG22	1:A:318:TYR:H	1.84	0.42
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.53	0.42
2:B:90:VAL:O	2:B:91:GLN:C	2.56	0.42
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.91	0.42
1:A:23:GLN:HG2	1:A:25:PRO:CD	2.48	0.42
1:A:389:PHE:CD1	1:A:391:LEU:HD21	2.54	0.42
1:A:411:ILE:HD12	1:A:412:PRO:CD	2.42	0.42
1:A:13:LYS:N	1:A:83:ARG:O	2.51	0.42
1:A:101:LYS:NZ	2:B:138:GLU:OE2	2.48	0.42
2:B:278:GLN:NE2	2:B:298:GLU:CB	2.74	0.42
2:B:76:ASP:O	2:B:76:ASP:CG	2.56	0.42
1:A:222:GLN:CG	1:A:223:LYS:H	2.16	0.42
2:B:105:SER:OG	2:B:235:HIS:CE1	2.72	0.42
2:B:324:ASP:O	2:B:343:GLN:HG2	2.20	0.42
1:A:100:LEU:O	1:A:318:TYR:HB3	2.20	0.42
1:A:156:SER:O	1:A:157:PRO:C	2.56	0.42
1:A:465:LYS:HE2	1:A:488:ASP:OD2	2.20	0.42
2:B:18:GLY:CA	2:B:127:TYR:CE1	3.03	0.42
2:B:302:GLU:HA	2:B:305:GLU:HB3	2.00	0.42
1:A:57:ASN:ND2	1:A:58:THR:H	2.18	0.42
1:A:62:ALA:HA	1:A:72:ARG:O	2.20	0.42
2:B:249:LYS:HB2	2:B:252:TRP:CZ3	2.55	0.42
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LYS:HG3	2:B:413:GLU:CB	2.50	0.42
1:A:183:TYR:CZ	1:A:230:MET:SD	3.13	0.42
1:A:41:MET:HB3	1:A:47:ILE:HG12	2.01	0.42
1:A:469:LEU:HD11	1:A:480:GLN:HG2	2.02	0.42
2:B:266:TRP:CD1	2:B:422:LEU:HD23	2.54	0.42
2:B:422:LEU:HD12	2:B:425:LEU:HD12	2.01	0.42
1:A:106:VAL:CG1	1:A:107:THR:N	2.74	0.42
1:A:162:SER:O	1:A:163:SER:C	2.58	0.42
1:A:542:ILE:CG2	1:A:543:GLY:N	2.83	0.42
1:A:445:ALA:HB2	1:A:549:ASP:OD1	2.20	0.42
2:B:312:GLU:CG	2:B:312:GLU:O	2.68	0.42
2:B:357:MET:H	2:B:357:MET:HG3	1.66	0.42
1:A:267:ALA:O	1:A:271:TYR:HB2	2.19	0.41
1:A:244:ILE:CD1	1:A:310:LEU:HD13	2.41	0.41
2:B:148:VAL:O	2:B:150:PRO:HD3	2.20	0.41
2:B:270:ILE:HG23	2:B:346:PHE:O	2.19	0.41
1:A:104:LYS:HB2	1:A:192:ASP:HA	2.01	0.41
1:A:492:GLU:HG2	1:A:530:LYS:HD2	2.02	0.41
2:B:17:ASP:O	2:B:83:ARG:NE	2.37	0.41
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.01	0.41
1:A:519:ASN:O	1:A:523:GLU:HG3	2.21	0.41
2:B:195:ILE:O	2:B:199:ARG:HG3	2.21	0.41
2:B:212:TRP:CE3	2:B:212:TRP:HA	2.55	0.41
2:B:306:ASN:HA	2:B:309:ILE:CG2	2.50	0.41
2:B:317:VAL:HG12	2:B:349:LEU:CD2	2.50	0.41
2:B:326:ILE:HB	2:B:342:TYR:CD1	2.55	0.41
2:B:345:PRO:C	2:B:346:PHE:CD1	2.94	0.41
2:B:395:LYS:HG2	2:B:399:GLU:OE1	2.21	0.41
2:B:90:VAL:HG12	2:B:91:GLN:N	2.34	0.41
1:A:30:LYS:O	1:A:31:ILE:C	2.59	0.41
1:A:344:GLU:HA	1:A:345:PRO:HD3	1.66	0.41
1:A:440:PHE:HE1	1:A:489:SER:CB	2.33	0.41
1:A:451:LYS:O	1:A:471:ASN:N	2.52	0.41
1:A:540:LYS:O	1:A:540:LYS:CG	2.66	0.41
2:B:235:HIS:HA	2:B:236:PRO:HD2	1.67	0.41
2:B:254:VAL:O	2:B:257:ILE:HG23	2.20	0.41
1:A:356:ARG:HH11	1:A:358:ARG:HD2	1.84	0.41
1:A:420:PRO:HA	1:A:421:PRO:C	2.40	0.41
1:A:506:ILE:CG2	1:A:533:LEU:HD12	2.44	0.41
2:B:246:LEU:HD21	2:B:310:LEU:HD11	2.02	0.41
2:B:298:GLU:O	2:B:301:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:CG	1:A:80:LEU:HA	2.50	0.41
2:B:200:THR:O	2:B:204:GLU:N	2.48	0.41
2:B:358:ARG:O	2:B:361:HIS:NE2	2.53	0.41
2:B:53:GLU:O	2:B:55:PRO:HD3	2.20	0.41
1:A:340:GLN:CB	1:A:351:THR:HG22	2.50	0.41
1:A:460:ASN:N	1:A:460:ASN:HD22	2.19	0.41
1:A:474:ASN:HD22	1:A:474:ASN:H	1.68	0.41
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.36	0.41
2:B:363:ASN:OD1	2:B:366:LYS:HB2	2.21	0.41
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.50	0.41
1:A:201:LYS:O	1:A:204:GLU:HB2	2.21	0.41
1:A:477:THR:O	1:A:480:GLN:N	2.51	0.41
1:A:77:PHE:O	1:A:78:ARG:C	2.58	0.41
2:B:296:THR:H	2:B:299:ALA:HB3	1.85	0.41
1:A:356:ARG:O	1:A:356:ARG:HG3	2.21	0.41
2:B:171:PHE:C	2:B:171:PHE:CD1	2.94	0.41
2:B:200:THR:O	2:B:202:ILE:N	2.54	0.41
2:B:31:ILE:HG22	2:B:35:VAL:HG21	2.03	0.41
2:B:366:LYS:HA	2:B:405:TYR:CD1	2.56	0.41
2:B:362:THR:CG2	2:B:366:LYS:NZ	2.84	0.41
2:B:370:GLU:O	2:B:371:ALA:C	2.58	0.41
1:A:12:LEU:CD1	1:A:127:TYR:CE1	3.04	0.41
1:A:22:LYS:HB2	1:A:22:LYS:HE2	1.89	0.41
1:A:395:LYS:HE2	1:A:399:GLU:OE1	2.21	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD2	1.82	0.41
2:B:16:MET:HG3	2:B:83:ARG:HG2	2.03	0.41
2:B:287:LYS:C	2:B:288:ALA:O	2.58	0.41
2:B:24:TRP:HZ3	2:B:59:PRO:CB	2.34	0.41
1:A:270:ILE:O	1:A:272:PRO:HD3	2.20	0.40
1:A:515:SER:O	1:A:517:LEU:N	2.54	0.40
1:A:88:TRP:HH2	2:B:22:LYS:HZ1	1.68	0.40
1:A:407:GLN:HG2	2:B:393:ILE:HA	2.03	0.40
2:B:65:LYS:HZ3	2:B:409:THR:CG2	2.33	0.40
1:A:172:LYS:HB3	1:A:172:LYS:HE2	1.70	0.40
1:A:17:ASP:O	1:A:83:ARG:CD	2.65	0.40
1:A:241:VAL:HG12	1:A:242:GLN:O	2.21	0.40
1:A:394:GLN:O	1:A:397:THR:N	2.52	0.40
1:A:536:VAL:HG11	1:A:542:ILE:CG1	2.51	0.40
1:A:535:TRP:C	1:A:536:VAL:HG23	2.42	0.40
2:B:54:ASN:ND2	2:B:126:LYS:HA	2.35	0.40
2:B:216:THR:N	2:B:217:PRO:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LYS:O	1:A:204:GLU:N	2.54	0.40
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.78	0.40
1:A:283:LEU:O	1:A:285:GLY:N	2.54	0.40
1:A:498:ASP:HA	1:A:536:VAL:O	2.21	0.40
2:B:245:VAL:HG12	2:B:246:LEU:O	2.22	0.40
2:B:330:GLN:CG	2:B:338:THR:HG1	2.34	0.40
1:A:342:TYR:C	1:A:342:TYR:CD1	2.94	0.40
1:A:31:ILE:O	1:A:35:VAL:HG23	2.21	0.40
1:A:3:SER:OG	1:A:5:ILE:HD12	2.21	0.40
1:A:535:TRP:O	1:A:536:VAL:HG23	2.21	0.40
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	3.09	0.40
1:A:3:SER:HB2	1:A:4:PRO:HD2	2.03	0.40
1:A:55:PRO:HB2	1:A:143:ARG:CZ	2.52	0.40
2:B:12:LEU:H	2:B:12:LEU:HD12	1.86	0.40
2:B:195:ILE:HG13	2:B:199:ARG:HG3	2.03	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	550/560 (98%)	428 (78%)	89 (16%)	33 (6%)	2	10
2	B	425/430 (99%)	329 (77%)	65 (15%)	31 (7%)	1	6
All	All	975/990 (98%)	757 (78%)	154 (16%)	64 (7%)	1	8

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	195	ILE
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	224	GLU
1	A	230	MET
1	A	515	SER
2	B	7	THR
2	B	68	SER
2	B	116	PHE
2	B	126	LYS
2	B	217	PRO
2	B	227	PHE
2	B	277	ARG
2	B	297	GLU
2	B	360	ALA
2	B	421	PRO
1	A	14	PRO
1	A	85	GLN
1	A	89	GLU
1	A	158	ALA
1	A	174	GLN
1	A	283	LEU
1	A	516	GLU
2	B	85	GLN
2	B	154	LYS
2	B	161	GLN
2	B	199	ARG
2	B	220	LYS
2	B	307	ARG
2	B	357	MET
2	B	359	GLY
2	B	365	VAL
1	A	28	GLU
1	A	52	PRO
1	A	276	VAL
1	A	397	THR
1	A	513	SER
1	A	538	ALA
2	B	18	GLY
2	B	77	PHE
2	B	137	ASN
2	B	229	TRP
2	B	419	THR
2	B	420	PRO
1	A	31	ILE

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Mol	Chain	Res	Type
1	A	69	THR
1	A	126	LYS
1	A	135	ILE
1	A	284	ARG
1	A	345	PRO
1	A	360	ALA
1	A	465	LYS
2	B	3	SER
2	B	194	GLU
1	A	122	GLU
1	A	123	ASP
1	A	471	ASN
1	A	503	LEU
2	B	175	ASN
1	A	148	VAL
1	A	356	ARG
2	B	243	PRO
2	B	5	ILE
2	B	372	VAL

### 5.3.2 Protein sidechains [i](#)

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	494/500 (99%)	452 (92%)	42 (8%)	12	43
2	B	389/392 (99%)	356 (92%)	33 (8%)	12	43
All	All	883/892 (99%)	808 (92%)	75 (8%)	12	43

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	26	LEU
1	A	40	GLU
1	A	49	LYS

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Mol	Chain	Res	Type
1	A	52	PRO
1	A	56	TYR
1	A	58	THR
1	A	65	LYS
1	A	71	TRP
1	A	104	LYS
1	A	136	ASN
1	A	138	GLU
1	A	142	ILE
1	A	161	GLN
1	A	162	SER
1	A	172	LYS
1	A	177	ASP
1	A	201	LYS
1	A	207	GLN
1	A	216	THR
1	A	228	LEU
1	A	269	GLN
1	A	274	ILE
1	A	300	GLU
1	A	315	HIS
1	A	326	ILE
1	A	347	LYS
1	A	364	ASP
1	A	391	LEU
1	A	394	GLN
1	A	397	THR
1	A	402	TRP
1	A	410	TRP
1	A	457	TYR
1	A	460	ASN
1	A	461	LYS
1	A	473	THR
1	A	499	SER
1	A	506	ILE
1	A	511	ASP
1	A	514	GLU
1	A	546	GLU
2	B	7	THR
2	B	16	MET
2	B	22	LYS
2	B	64	LYS

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Mol	Chain	Res	Type
2	B	67	ASP
2	B	70	LYS
2	B	109	LEU
2	B	113	ASP
2	B	134	SER
2	B	163	SER
2	B	170	PRO
2	B	177	ASP
2	B	193	LEU
2	B	212	TRP
2	B	221	HIS
2	B	229	TRP
2	B	232	TYR
2	B	239	TRP
2	B	244	ILE
2	B	246	LEU
2	B	250	ASP
2	B	252	TRP
2	B	277	ARG
2	B	279	LEU
2	B	294	PRO
2	B	305	GLU
2	B	330	GLN
2	B	336	GLN
2	B	338	THR
2	B	340	GLN
2	B	342	TYR
2	B	374	LYS
2	B	399	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	91	GLN
1	A	96	HIS
1	A	136	ASN
1	A	137	ASN
1	A	151	GLN
1	A	161	GLN
1	A	235	HIS
1	A	242	GLN

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Mol	Chain	Res	Type
1	A	255	ASN
1	A	269	GLN
1	A	340	GLN
1	A	367	GLN
1	A	394	GLN
1	A	460	ASN
1	A	474	ASN
1	A	475	GLN
1	A	487	GLN
1	A	494	ASN
1	A	507	GLN
1	A	509	GLN
2	B	23	GLN
2	B	136	ASN
2	B	174	GLN
2	B	182	GLN
2	B	207	GLN
2	B	258	GLN
2	B	367	GLN
2	B	373	GLN
2	B	394	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 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	TPB	A	701	-	27,27,27	3.25	16 (59%)	36,37,37	2.32	10 (27%)

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	TPB	A	701	-	-	0/10/10/10	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	TPB	C11-N5	2.06	1.45	1.40
3	A	701	TPB	C61-C6	2.22	1.55	1.51
3	A	701	TPB	C12-C11	2.32	1.43	1.39
3	A	701	TPB	C1-C2	3.05	1.44	1.40
3	A	701	TPB	C15-C14	3.22	1.46	1.39
3	A	701	TPB	C13-C12	3.64	1.45	1.38
3	A	701	TPB	C16-C15	3.65	1.45	1.38
3	A	701	TPB	C3-C2	3.68	1.45	1.39
3	A	701	TPB	C9-N5	3.99	1.44	1.36
3	A	701	TPB	C1-C6	4.17	1.46	1.40
3	A	701	TPB	C5-C4	4.36	1.46	1.39
3	A	701	TPB	C8-N7	4.46	1.46	1.38
3	A	701	TPB	C16-C11	4.56	1.46	1.39
3	A	701	TPB	C10-N3	4.91	1.45	1.34
3	A	701	TPB	C5-C6	5.04	1.47	1.39
3	A	701	TPB	C9-N3	7.59	1.44	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	TPB	N3-C9-N1	-9.28	117.75	126.68
3	A	701	TPB	C1-N7-C8	-3.58	117.71	124.05
3	A	701	TPB	C7-C10-N3	-3.19	120.24	123.92
3	A	701	TPB	C13-C14-C17	-2.29	116.16	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	TPB	C3-C2-C1	2.07	120.64	118.18
3	A	701	TPB	C15-C14-C17	2.37	123.96	119.99
3	A	701	TPB	C6-C1-N7	2.82	124.03	119.27
3	A	701	TPB	C61-C6-C1	2.84	125.03	121.41
3	A	701	TPB	C10-N3-C9	3.36	118.23	115.43
3	A	701	TPB	C9-N1-C8	4.02	123.56	116.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	TPB	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	552/560 (98%)	-0.20	16 (2%)	52	24	49, 95, 121, 122	18 (3%)
2	B	427/430 (99%)	-0.18	15 (3%)	44	19	32, 80, 121, 122	7 (1%)
All	All	979/990 (98%)	-0.19	31 (3%)	48	21	32, 90, 121, 122	25 (2%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	HIS	7.7
1	A	549	ASP	5.7
2	B	226	PRO	4.2
1	A	1	PRO	4.1
1	A	142	ILE	3.5
1	A	444	GLY	3.5
2	B	222	GLN	3.4
1	A	141	GLY	3.1
1	A	547	GLN	3.0
1	A	134	SER	3.0
2	B	2	ILE	3.0
2	B	3	SER	3.0
1	A	140	PRO	2.9
1	A	220	LYS	2.8
1	A	360	ALA	2.8
2	B	299	ALA	2.7
2	B	225	PRO	2.6
1	A	133	PRO	2.6
2	B	231	GLY	2.5
1	A	455	ALA	2.4
2	B	297	GLU	2.2
1	A	138	GLU	2.2
2	B	279	LEU	2.2
2	B	306	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	286	THR	2.1
2	B	305	GLU	2.1
2	B	229	TRP	2.1
2	B	296	THR	2.1
2	B	409	THR	2.1
2	B	224	GLU	2.1
1	A	551	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	TPB	A	701	25/25	0.93	0.47	3.10	55,70,77,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.