



Full wwPDB X-ray Structure Validation Report i

Oct 16, 2021 – 11:34 PM EDT

PDB ID : 1S9G
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN COMPLEX WITH JANSSEN-R120394.
Authors : Das, K.; Clark Jr., A.D.; Ludovici, D.W.; Kukla, M.J.; Decorte, B.; Lewi, P.J.; Hughes, S.H.; Janssen, P.A.; Arnold, E.
Deposited on : 2004-02-04
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

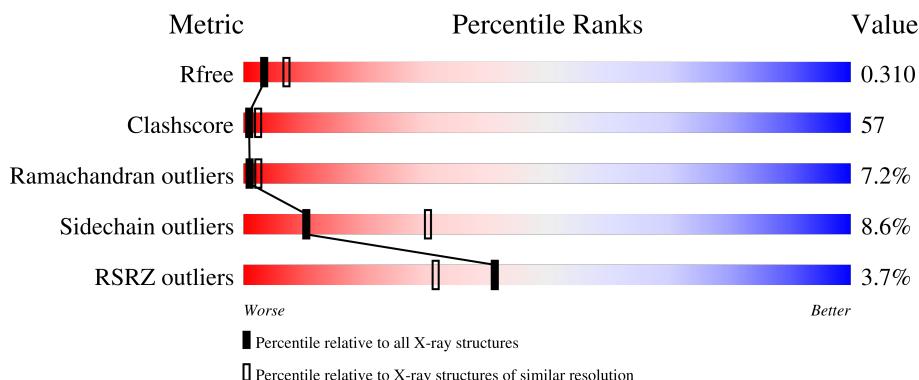
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

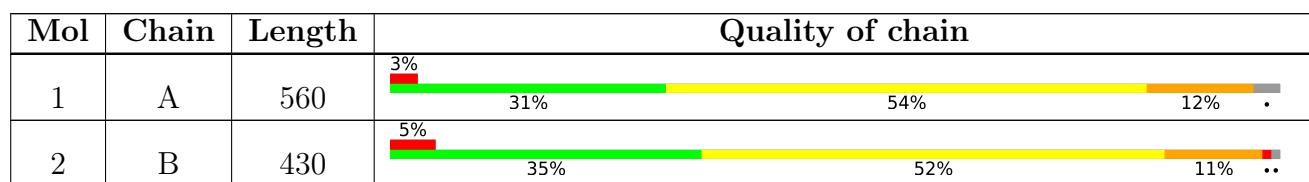
The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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.



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	ABZ	A	701	-	-	X	-

2 Entry composition [\(i\)](#)

There are 4 unique types of molecules in this entry. The entry contains 8112 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
			Total	C	N	O	S			
1	A	543	4429	2871	736	815	7	66	0	0

There is a discrepancy between the modelled and reference sequences:

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

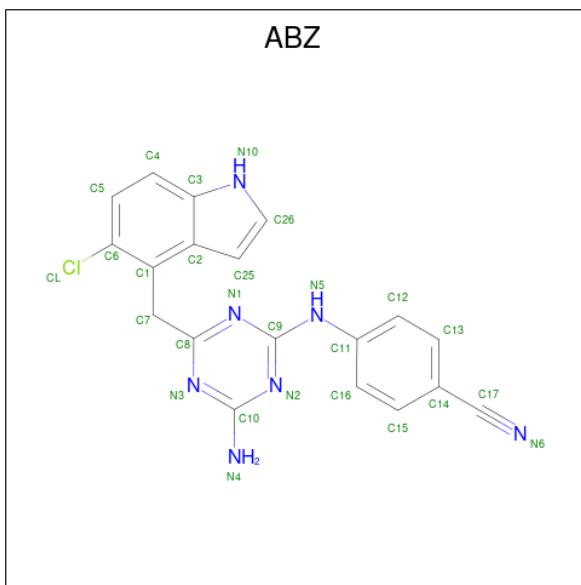
- Molecule 2 is a protein called POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	425	3514	2289	582	636	7	55	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is 4-[4-AMINO-6-(5-CHLORO-1H-INDOL-4-YLMETHYL)-[1,3,5]TRIAZIN-2-YLAMINO]-BENZONITRILE (three-letter code: ABZ) (formula: C₁₉H₁₄ClN₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 27	C 19	Cl 1	N 7	0	0

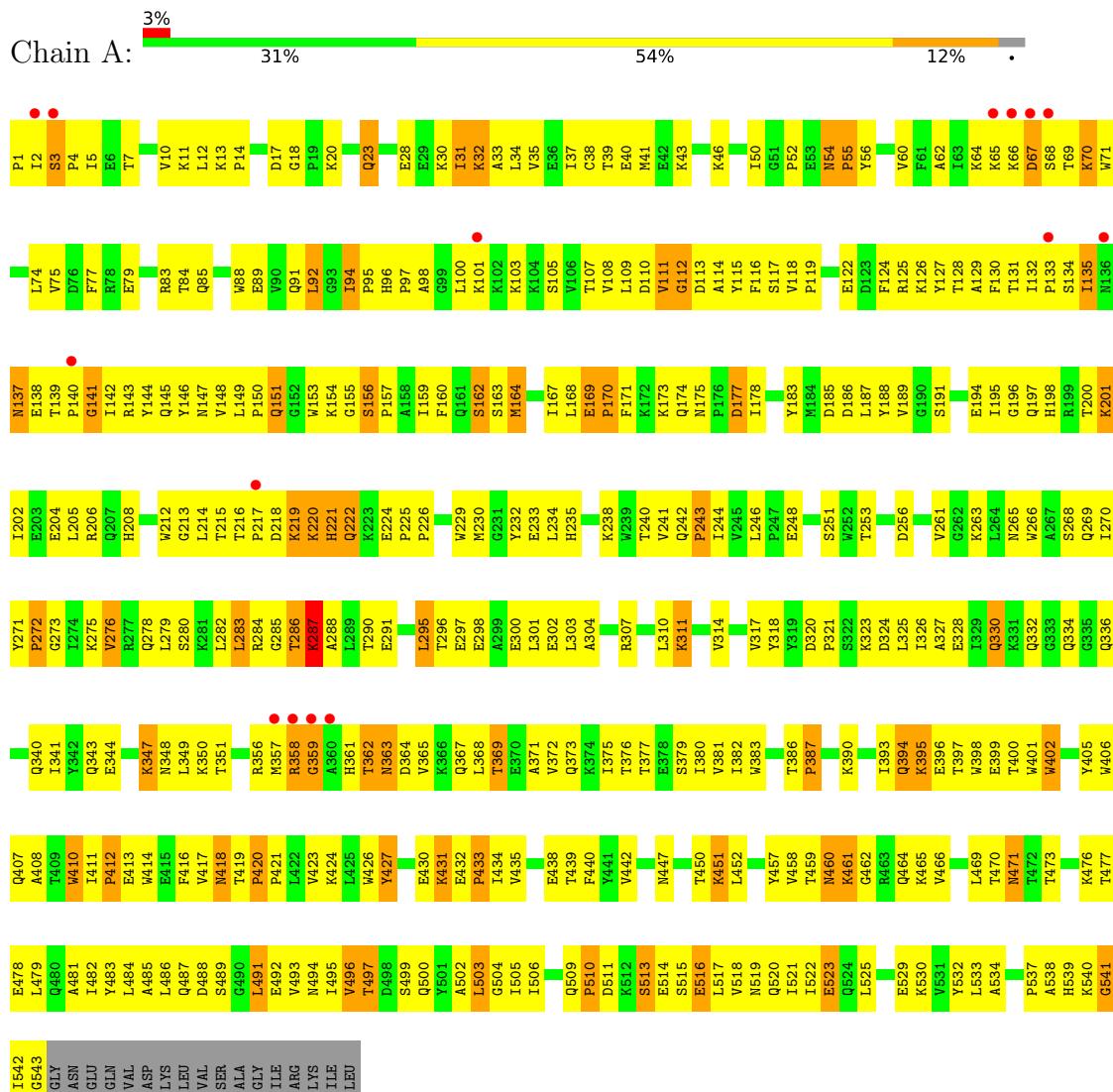
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total 79		O 79	0
4	B	63	Total 63		O 63	0

3 Residue-property plots

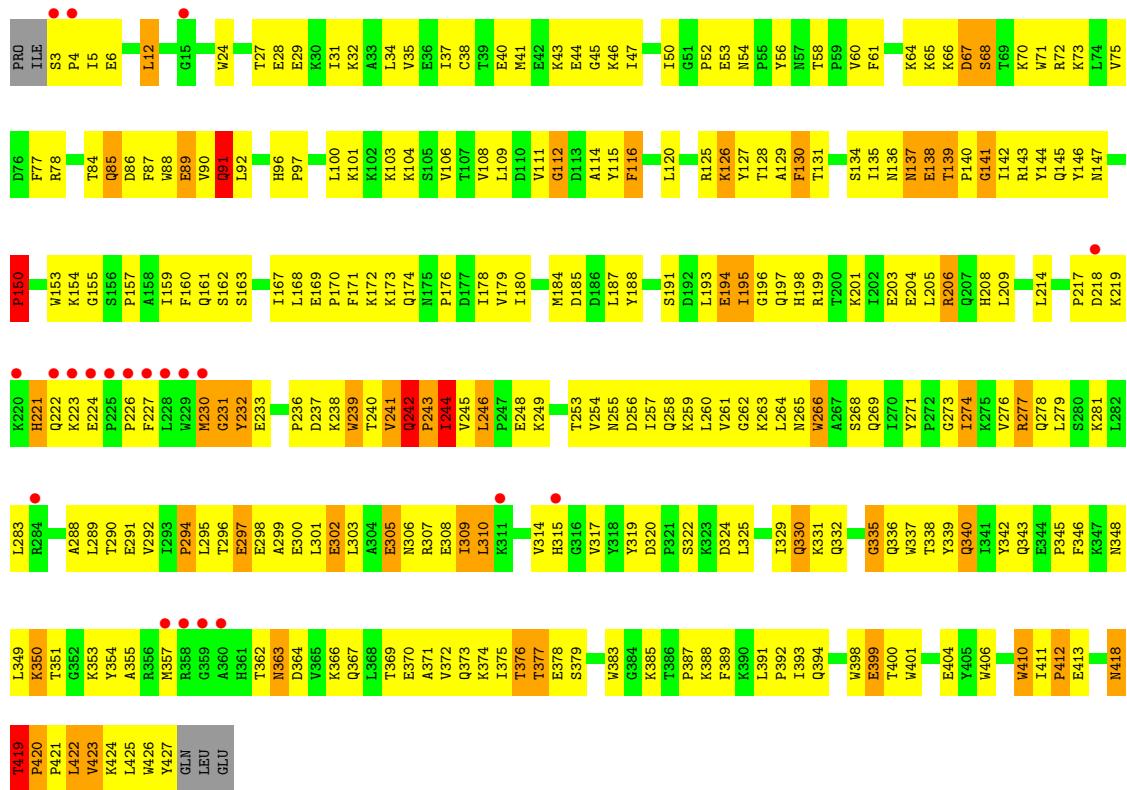
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.60Å 68.60Å 103.00Å 90.00° 107.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 25.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-2.80) 91.9 (25.21-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.25 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R , R_{free}	0.242 , 0.312 0.246 , 0.310	Depositor DCC
R_{free} test set	1726 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8112	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.53	0/4547	0.83	4/6178 (0.1%)
2	B	0.64	0/3618	0.90	5/4918 (0.1%)
All	All	0.58	0/8165	0.86	9/11096 (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
2	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ASN	N-CA-C	-7.76	90.06	111.00
1	A	359	GLY	N-CA-C	-7.62	94.05	113.10
1	A	286	THR	N-CA-C	-7.56	90.60	111.00
2	B	89	GLU	N-CA-C	-6.43	93.64	111.00
2	B	230	MET	N-CA-C	6.23	127.82	111.00
1	A	92	LEU	CB-CG-CD1	-5.53	101.60	111.00
2	B	244	ILE	N-CA-C	-5.45	96.28	111.00
2	B	194	GLU	N-CA-C	-5.21	96.94	111.00
2	B	423	VAL	N-CA-C	-5.20	96.95	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	PHE	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	4429	0	4491	524	0
2	B	3514	0	3547	403	0
3	A	27	0	14	11	0
4	A	79	0	0	3	0
4	B	63	0	0	2	0
All	All	8112	0	8052	893	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 57.

All (893) 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:297:GLU:HG2	2:B:298:GLU:N	1.56	1.13
1:A:2:ILE:HG21	1:A:5:ILE:HG13	1.31	1.12
2:B:206:ARG:HB3	2:B:206:ARG:NH1	1.64	1.11
2:B:297:GLU:HG2	2:B:298:GLU:H	0.95	1.10
1:A:311:LYS:HA	1:A:311:LYS:CE	1.82	1.09
1:A:311:LYS:HA	1:A:311:LYS:HE3	1.08	1.08
1:A:460:ASN:ND2	1:A:461:LYS:H	1.51	1.08
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.16	1.06
1:A:1:PRO:HG2	1:A:117:SER:HA	1.37	1.02
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.24	1.02
1:A:494:ASN:HD22	2:B:289:LEU:HD12	1.21	1.01
2:B:371:ALA:O	2:B:375:ILE:HG13	1.60	1.01
1:A:460:ASN:HD22	1:A:461:LYS:H	1.07	1.00
1:A:435:VAL:HG12	2:B:290:THR:HG21	1.40	0.98
1:A:542:ILE:HG12	1:A:543:GLY:H	1.26	0.98
1:A:3:SER:H	1:A:4:PRO:HD2	1.28	0.97
1:A:406:TRP:CE3	2:B:420:PRO:HG2	1.99	0.97
1:A:54:ASN:HD21	1:A:129:ALA:HB2	1.28	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:O	1:A:35:VAL:HG23	1.66	0.96
2:B:244:ILE:O	2:B:310:LEU:HD21	1.66	0.96
2:B:363:ASN:HD21	2:B:366:LYS:H	1.00	0.96
1:A:317:VAL:HG12	1:A:348:ASN:O	1.66	0.95
2:B:206:ARG:HB3	2:B:206:ARG:HH11	1.21	0.95
1:A:84:THR:HG22	1:A:124:PHE:CZ	2.01	0.95
2:B:297:GLU:CG	2:B:298:GLU:H	1.79	0.95
2:B:253:THR:HG22	2:B:292:VAL:HG22	1.48	0.94
1:A:283:LEU:C	1:A:285:GLY:H	1.62	0.94
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.50	0.94
1:A:2:ILE:HG22	1:A:5:ILE:H	1.31	0.93
1:A:311:LYS:HE3	1:A:311:LYS:CA	1.93	0.93
1:A:2:ILE:HG23	1:A:4:PRO:HG2	1.49	0.92
1:A:50:ILE:HD13	1:A:54:ASN:HD22	1.33	0.92
1:A:2:ILE:CG2	1:A:4:PRO:HG2	1.99	0.92
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.04	0.92
1:A:96:HIS:HD2	1:A:98:ALA:H	1.01	0.92
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.51	0.92
1:A:285:GLY:C	1:A:287:LYS:H	1.74	0.91
2:B:242:GLN:H	2:B:243:PRO:HD3	1.33	0.90
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.70	0.90
1:A:28:GLU:O	1:A:31:ILE:HG23	1.71	0.89
1:A:3:SER:N	1:A:4:PRO:HD2	1.86	0.89
1:A:311:LYS:CE	1:A:311:LYS:CA	2.51	0.88
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.55	0.88
2:B:240:THR:HG22	2:B:241:VAL:H	1.39	0.88
2:B:297:GLU:CG	2:B:298:GLU:N	2.28	0.88
1:A:134:SER:O	1:A:138:GLU:HB3	1.75	0.87
1:A:311:LYS:HE2	1:A:311:LYS:O	1.74	0.87
1:A:206:ARG:CZ	1:A:219:LYS:HA	2.05	0.86
1:A:438:GLU:HG3	1:A:460:ASN:HD21	1.39	0.86
2:B:254:VAL:O	2:B:258:GLN:HG3	1.74	0.86
2:B:363:ASN:C	2:B:363:ASN:HD22	1.78	0.86
1:A:96:HIS:CD2	1:A:98:ALA:H	1.91	0.86
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.10	0.84
1:A:178:ILE:HD11	1:A:201:LYS:HG3	1.59	0.84
1:A:132:ILE:HG23	1:A:142:ILE:HB	1.59	0.84
1:A:282:LEU:HD21	1:A:296:THR:HG23	1.56	0.84
1:A:482:ILE:HD11	1:A:497:THR:HG21	1.58	0.84
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.58	0.84
1:A:491:LEU:HD12	1:A:491:LEU:H	1.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:O	1:A:41:MET:HB2	1.78	0.83
1:A:460:ASN:HD22	1:A:461:LYS:N	1.74	0.83
1:A:452:LEU:HD23	1:A:470:THR:HA	1.58	0.82
2:B:231:GLY:O	2:B:233:GLU:N	2.12	0.82
2:B:363:ASN:ND2	2:B:366:LYS:H	1.76	0.82
1:A:244:ILE:HD11	1:A:310:LEU:HD22	1.61	0.81
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.61	0.81
2:B:301:LEU:O	2:B:305:GLU:HB3	1.80	0.81
2:B:163:SER:O	2:B:167:ILE:HG13	1.79	0.81
2:B:362:THR:CG2	2:B:367:GLN:HE21	1.92	0.81
1:A:54:ASN:ND2	1:A:129:ALA:HB2	1.96	0.80
1:A:132:ILE:CG2	1:A:142:ILE:HB	2.11	0.80
1:A:362:THR:HG21	1:A:367:GLN:HG3	1.62	0.80
2:B:84:THR:O	2:B:86:ASP:N	2.15	0.80
1:A:450:THR:O	1:A:451:LYS:HG3	1.83	0.79
1:A:442:VAL:HG22	1:A:481:ALA:HB1	1.62	0.79
1:A:542:ILE:HG12	1:A:543:GLY:N	1.96	0.79
1:A:362:THR:CG2	1:A:367:GLN:HG3	2.13	0.79
2:B:241:VAL:HG22	2:B:243:PRO:HD2	1.65	0.78
1:A:283:LEU:O	1:A:285:GLY:N	2.13	0.78
1:A:1:PRO:CG	1:A:117:SER:HA	2.12	0.78
2:B:303:LEU:HD21	2:B:307:ARG:NH1	1.98	0.78
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.66	0.77
1:A:283:LEU:C	1:A:285:GLY:N	2.32	0.77
2:B:242:GLN:N	2:B:243:PRO:HD3	2.00	0.77
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.67	0.77
1:A:198:HIS:O	1:A:202:ILE:HG12	1.84	0.77
1:A:285:GLY:C	1:A:287:LYS:N	2.37	0.77
1:A:66:LYS:NZ	1:A:66:LYS:HB3	2.00	0.77
1:A:411:ILE:HG13	1:A:411:ILE:O	1.85	0.77
2:B:203:GLU:HA	2:B:206:ARG:HB2	1.66	0.77
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.66	0.76
2:B:195:ILE:HG13	2:B:196:GLY:H	1.49	0.76
1:A:31:ILE:CD1	1:A:133:PRO:O	2.33	0.76
1:A:5:ILE:HD11	1:A:167:ILE:HD11	1.66	0.76
1:A:96:HIS:CE1	1:A:350:LYS:HE2	2.19	0.76
1:A:398:TRP:HE1	1:A:411:ILE:HG21	1.51	0.76
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.21	0.76
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.68	0.76
1:A:326:ILE:HD12	1:A:326:ILE:N	2.01	0.75
1:A:23:GLN:HE22	1:A:60:VAL:HG23	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG22	1:A:318:TYR:N	2.00	0.75
1:A:284:ARG:HE	1:A:358:ARG:HH12	1.34	0.75
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.50	0.75
2:B:31:ILE:O	2:B:35:VAL:HG23	1.87	0.75
1:A:296:THR:O	1:A:300:GLU:HG3	1.86	0.75
1:A:137:ASN:O	1:A:137:ASN:ND2	2.18	0.75
2:B:305:GLU:O	2:B:308:GLU:HG2	1.86	0.75
1:A:431:LYS:CD	1:A:431:LYS:H	2.00	0.74
1:A:206:ARG:NH2	1:A:219:LYS:HG3	2.02	0.74
1:A:112:GLY:O	1:A:114:ALA:N	2.21	0.74
1:A:406:TRP:CZ2	2:B:420:PRO:HD2	2.22	0.74
1:A:460:ASN:ND2	1:A:461:LYS:N	2.31	0.74
1:A:377:THR:O	1:A:381:VAL:HG23	1.88	0.74
2:B:195:ILE:HG13	2:B:196:GLY:N	2.02	0.74
1:A:135:ILE:HG22	1:A:135:ILE:O	1.87	0.74
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.87	0.74
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.68	0.74
1:A:324:ASP:HB2	1:A:326:ILE:HD11	1.70	0.73
1:A:2:ILE:HD12	1:A:5:ILE:HD12	1.68	0.73
1:A:431:LYS:H	1:A:431:LYS:CE	2.01	0.73
1:A:31:ILE:HD13	1:A:133:PRO:O	1.88	0.73
1:A:398:TRP:NE1	1:A:411:ILE:HG21	2.04	0.73
2:B:332:GLN:HA	2:B:332:GLN:OE1	1.87	0.72
2:B:363:ASN:HD21	2:B:366:LYS:N	1.83	0.72
1:A:244:ILE:HD11	1:A:310:LEU:HD13	1.70	0.72
2:B:58:THR:HG21	2:B:77:PHE:CE1	2.24	0.72
1:A:457:TYR:CE1	1:A:465:LYS:HB3	2.24	0.72
2:B:206:ARG:HH11	2:B:206:ARG:CB	2.00	0.72
2:B:303:LEU:HA	2:B:306:ASN:ND2	2.04	0.72
1:A:206:ARG:HH22	1:A:219:LYS:HG3	1.54	0.72
2:B:422:LEU:HB3	2:B:425:LEU:CD1	2.20	0.72
1:A:470:THR:O	1:A:471:ASN:HB3	1.88	0.72
1:A:3:SER:N	1:A:4:PRO:CD	2.51	0.72
1:A:64:LYS:HE3	1:A:68:SER:CB	2.19	0.72
1:A:317:VAL:HG22	1:A:318:TYR:H	1.54	0.72
1:A:28:GLU:O	1:A:31:ILE:CG2	2.38	0.72
1:A:188:TYR:CB	3:A:701:ABZ:H72	2.20	0.72
2:B:274:ILE:HD11	2:B:309:ILE:HG12	1.71	0.72
1:A:28:GLU:HA	1:A:31:ILE:CG2	2.20	0.71
1:A:132:ILE:HG22	1:A:142:ILE:O	1.90	0.71
1:A:2:ILE:O	1:A:119:PRO:HG3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:ILE:HG22	2:B:330:GLN:N	2.03	0.71
1:A:54:ASN:O	1:A:56:TYR:N	2.23	0.71
2:B:246:LEU:HD23	2:B:246:LEU:N	2.05	0.71
2:B:419:THR:O	2:B:421:PRO:HD3	1.91	0.71
1:A:2:ILE:HG22	1:A:5:ILE:N	2.03	0.71
1:A:96:HIS:HD2	1:A:98:ALA:N	1.83	0.71
1:A:382:ILE:O	2:B:136:ASN:HB2	1.92	0.70
1:A:419:THR:HG23	1:A:419:THR:O	1.91	0.70
2:B:12:LEU:HD12	2:B:12:LEU:H	1.56	0.70
2:B:274:ILE:HG21	2:B:306:ASN:CB	2.21	0.70
2:B:240:THR:HG22	2:B:241:VAL:N	2.07	0.70
1:A:398:TRP:CZ2	1:A:411:ILE:HG22	2.26	0.70
1:A:284:ARG:NE	1:A:358:ARG:HH12	1.88	0.70
1:A:398:TRP:HZ2	1:A:411:ILE:HG22	1.57	0.70
2:B:12:LEU:HD11	2:B:127:TYR:CE2	2.27	0.70
2:B:366:LYS:O	2:B:370:GLU:HG3	1.91	0.70
2:B:131:THR:OG1	2:B:143:ARG:NH1	2.24	0.69
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.57	0.69
2:B:240:THR:O	2:B:241:VAL:HB	1.92	0.69
1:A:452:LEU:CD2	1:A:470:THR:HA	2.23	0.69
2:B:199:ARG:HH12	2:B:230:MET:HE3	1.57	0.69
1:A:91:GLN:O	1:A:91:GLN:HG2	1.92	0.69
2:B:332:GLN:HB2	2:B:336:GLN:O	1.91	0.69
1:A:33:ALA:O	1:A:37:ILE:HG12	1.93	0.69
1:A:148:VAL:O	1:A:150:PRO:HD3	1.93	0.69
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.74	0.69
2:B:244:ILE:HB	2:B:310:LEU:HD21	1.75	0.69
2:B:274:ILE:HD12	2:B:306:ASN:HB2	1.74	0.68
1:A:397:THR:HG21	1:A:424:LYS:HA	1.74	0.68
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.23	0.68
1:A:420:PRO:HA	1:A:421:PRO:C	2.13	0.68
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.58	0.68
1:A:28:GLU:HA	1:A:31:ILE:HG22	1.76	0.68
2:B:203:GLU:HG3	2:B:203:GLU:O	1.91	0.68
2:B:303:LEU:HD21	2:B:307:ARG:HH12	1.58	0.68
1:A:540:LYS:HG3	1:A:541:GLY:N	2.09	0.68
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.58	0.68
2:B:274:ILE:HG21	2:B:306:ASN:HB2	1.74	0.68
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.59	0.68
1:A:368:LEU:O	1:A:372:VAL:HG23	1.94	0.67
2:B:369:THR:O	2:B:373:GLN:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ILE:HD13	2:B:283:LEU:HG	1.75	0.67
1:A:362:THR:HG22	1:A:367:GLN:HE21	1.58	0.67
1:A:344:GLU:OE1	1:A:344:GLU:HA	1.94	0.67
1:A:431:LYS:H	1:A:431:LYS:HE2	1.59	0.67
1:A:131:THR:OG1	1:A:143:ARG:HG3	1.94	0.67
1:A:235:HIS:HB2	1:A:238:LYS:HG3	1.77	0.67
2:B:329:ILE:HG22	2:B:330:GLN:H	1.57	0.67
1:A:398:TRP:CZ2	1:A:411:ILE:CG2	2.77	0.67
1:A:110:ASP:HB3	1:A:218:ASP:CG	2.16	0.66
1:A:215:THR:HG22	1:A:216:THR:N	2.10	0.66
1:A:101:LYS:O	1:A:103:LYS:HG2	1.94	0.66
1:A:20:LYS:HG2	1:A:55:PRO:O	1.96	0.66
2:B:253:THR:HA	2:B:292:VAL:HA	1.78	0.66
2:B:298:GLU:HG3	2:B:301:LEU:CD1	2.25	0.66
1:A:64:LYS:HE3	1:A:68:SER:HB2	1.76	0.66
1:A:451:LYS:HD3	1:A:471:ASN:HA	1.76	0.66
2:B:3:SER:N	2:B:4:PRO:HD3	2.11	0.65
1:A:111:VAL:HA	1:A:216:THR:HG22	1.76	0.65
1:A:406:TRP:CH2	2:B:420:PRO:HD2	2.32	0.65
1:A:191:SER:OG	1:A:198:HIS:ND1	2.28	0.65
1:A:486:LEU:HD23	1:A:495:ILE:HD11	1.79	0.65
1:A:518:VAL:O	1:A:522:ILE:HG13	1.97	0.65
1:A:69:THR:O	1:A:70:LYS:HD3	1.97	0.65
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.32	0.65
1:A:188:TYR:HB3	3:A:701:ABZ:H72	1.77	0.64
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.32	0.64
1:A:431:LYS:HD3	1:A:431:LYS:N	2.12	0.64
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.78	0.64
1:A:17:ASP:O	1:A:83:ARG:HD3	1.97	0.64
2:B:421:PRO:C	2:B:423:VAL:H	2.00	0.64
1:A:361:HIS:ND1	1:A:505:ILE:HD12	2.13	0.64
1:A:96:HIS:H	2:B:136:ASN:HD21	1.46	0.64
1:A:371:ALA:O	1:A:375:ILE:HG13	1.97	0.64
2:B:421:PRO:O	2:B:423:VAL:N	2.26	0.64
2:B:419:THR:H	2:B:420:PRO:HD3	1.62	0.64
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.32	0.64
2:B:101:LYS:O	2:B:236:PRO:HB2	1.97	0.63
2:B:257:ILE:HG23	2:B:258:GLN:H	1.62	0.63
1:A:101:LYS:HD3	1:A:103:LYS:HZ1	1.61	0.63
2:B:243:PRO:C	2:B:245:VAL:H	2.02	0.63
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:HG3	1:A:466:VAL:N	2.14	0.63
2:B:115:TYR:OH	2:B:184:MET:O	2.17	0.63
2:B:242:GLN:N	2:B:243:PRO:CD	2.61	0.63
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.34	0.63
1:A:3:SER:H	1:A:4:PRO:CD	2.06	0.63
1:A:253:THR:O	1:A:256:ASP:HB2	1.99	0.62
2:B:134:SER:HB3	2:B:139:THR:HG22	1.81	0.62
1:A:361:HIS:CE1	1:A:505:ILE:HD12	2.34	0.62
1:A:431:LYS:CD	1:A:431:LYS:N	2.63	0.62
2:B:27:THR:HG22	2:B:29:GLU:H	1.64	0.62
2:B:278:GLN:HG3	2:B:299:ALA:HA	1.81	0.62
1:A:122:GLU:O	1:A:125:ARG:HB2	1.99	0.62
2:B:244:ILE:HD12	2:B:310:LEU:O	1.99	0.62
1:A:197:GLN:O	1:A:200:THR:N	2.32	0.62
2:B:199:ARG:HH12	2:B:230:MET:CE	2.13	0.62
2:B:85:GLN:HB2	2:B:154:LYS:HB2	1.80	0.62
2:B:248:GLU:HA	2:B:307:ARG:NH2	2.14	0.62
2:B:257:ILE:HG12	2:B:283:LEU:HD11	1.80	0.62
1:A:430:GLU:O	1:A:532:TYR:HD2	1.82	0.61
2:B:224:GLU:O	2:B:226:PRO:HD3	2.00	0.61
2:B:331:LYS:HZ1	2:B:364:ASP:CG	2.02	0.61
1:A:2:ILE:HD12	1:A:5:ILE:CD1	2.30	0.61
1:A:50:ILE:HD13	1:A:54:ASN:ND2	2.11	0.61
1:A:69:THR:C	1:A:70:LYS:HD3	2.21	0.61
2:B:231:GLY:HA3	2:B:233:GLU:OE2	1.99	0.61
1:A:151:GLN:O	1:A:151:GLN:HG2	1.99	0.61
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.82	0.61
2:B:308:GLU:CG	2:B:309:ILE:N	2.63	0.61
2:B:363:ASN:C	2:B:363:ASN:ND2	2.49	0.61
1:A:178:ILE:HD11	1:A:201:LYS:CG	2.31	0.61
1:A:248:GLU:HG2	1:A:307:ARG:NH2	2.15	0.61
1:A:494:ASN:ND2	2:B:289:LEU:HD12	2.05	0.61
2:B:66:LYS:O	2:B:68:SER:N	2.33	0.61
1:A:125:ARG:HE	1:A:147:ASN:HA	1.66	0.61
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.36	0.61
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.82	0.61
1:A:77:PHE:CE1	1:A:150:PRO:HB3	2.36	0.61
1:A:532:TYR:CE1	1:A:534:ALA:HB2	2.36	0.61
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.31	0.61
1:A:290:THR:O	1:A:290:THR:HG22	2.01	0.60
1:A:397:THR:O	1:A:400:THR:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:THR:O	2:B:87:PHE:N	2.23	0.60
1:A:376:THR:HG23	1:A:386:THR:HG22	1.81	0.60
1:A:537:PRO:O	1:A:541:GLY:HA3	2.02	0.60
2:B:53:GLU:OE1	2:B:53:GLU:N	2.30	0.60
2:B:231:GLY:C	2:B:233:GLU:H	2.04	0.60
2:B:274:ILE:CD1	2:B:306:ASN:HB2	2.31	0.60
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.65	0.60
1:A:431:LYS:H	1:A:431:LYS:HD3	1.65	0.60
2:B:373:GLN:NE2	2:B:406:TRP:HA	2.16	0.60
1:A:39:THR:O	1:A:43:LYS:HB2	2.02	0.60
2:B:422:LEU:HB3	2:B:425:LEU:HG	1.83	0.60
1:A:56:TYR:O	1:A:129:ALA:HB3	2.02	0.59
2:B:115:TYR:HE1	2:B:185:ASP:OD1	1.85	0.59
2:B:217:PRO:O	2:B:219:LYS:N	2.30	0.59
1:A:343:GLN:HG3	1:A:349:LEU:HD22	1.84	0.59
2:B:199:ARG:NH1	2:B:230:MET:HE3	2.18	0.59
2:B:314:VAL:HG22	2:B:315:HIS:N	2.16	0.59
2:B:345:PRO:HB2	2:B:346:PHE:CE1	2.36	0.59
2:B:376:THR:O	2:B:379:SER:N	2.34	0.59
2:B:418:ASN:N	2:B:418:ASN:ND2	2.50	0.59
2:B:137:ASN:C	2:B:139:THR:H	2.06	0.59
2:B:266:TRP:CZ3	2:B:269:GLN:HB2	2.37	0.59
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.68	0.59
1:A:30:LYS:HA	1:A:33:ALA:HB3	1.84	0.59
1:A:540:LYS:HD2	2:B:265:ASN:ND2	2.18	0.59
2:B:27:THR:HG22	2:B:29:GLU:HB3	1.83	0.59
2:B:112:GLY:HA3	2:B:185:ASP:HB3	1.83	0.59
2:B:237:ASP:OD1	2:B:238:LYS:HG2	2.03	0.59
1:A:244:ILE:HD11	1:A:310:LEU:CD2	2.32	0.59
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.32	0.59
1:A:406:TRP:CZ3	2:B:420:PRO:HG2	2.37	0.59
2:B:297:GLU:C	2:B:299:ALA:H	2.06	0.59
2:B:419:THR:N	2:B:420:PRO:CD	2.66	0.59
1:A:540:LYS:HG3	1:A:541:GLY:H	1.66	0.58
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.67	0.58
1:A:284:ARG:CD	1:A:358:ARG:HH12	2.16	0.58
2:B:231:GLY:C	2:B:233:GLU:N	2.56	0.58
1:A:108:VAL:HG22	1:A:109:LEU:N	2.17	0.58
1:A:398:TRP:HE1	1:A:411:ILE:HD13	1.67	0.58
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.84	0.58
2:B:27:THR:CG2	2:B:29:GLU:HB3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.38	0.58
2:B:259:LYS:HB3	2:B:263:LYS:NZ	2.19	0.58
2:B:426:TRP:O	2:B:426:TRP:HD1	1.86	0.58
1:A:2:ILE:O	1:A:119:PRO:CG	2.51	0.58
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.38	0.58
1:A:140:PRO:O	1:A:141:GLY:O	2.21	0.58
1:A:270:ILE:O	1:A:272:PRO:HD3	2.04	0.58
1:A:356:ARG:HH12	1:A:359:GLY:HA3	1.68	0.58
1:A:411:ILE:O	1:A:411:ILE:CG1	2.52	0.58
2:B:278:GLN:HG2	2:B:298:GLU:C	2.23	0.58
1:A:317:VAL:CG2	1:A:318:TYR:N	2.67	0.58
1:A:410:TRP:HD1	2:B:401:TRP:CD2	2.21	0.58
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.34	0.57
1:A:125:ARG:HG2	1:A:146:TYR:O	2.03	0.57
2:B:332:GLN:CG	2:B:338:THR:HG23	2.31	0.57
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.86	0.57
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.39	0.57
2:B:37:ILE:O	2:B:41:MET:HG3	2.03	0.57
2:B:259:LYS:O	2:B:262:GLY:N	2.35	0.57
1:A:217:PRO:HA	1:A:219:LYS:NZ	2.19	0.57
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.68	0.57
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.85	0.57
1:A:276:VAL:HG12	1:A:276:VAL:O	2.02	0.57
1:A:317:VAL:CG2	1:A:318:TYR:H	2.16	0.57
1:A:478:GLU:OE2	1:A:499:SER:CB	2.53	0.57
1:A:495:ILE:HB	1:A:533:LEU:HD23	1.87	0.57
2:B:206:ARG:HB3	2:B:206:ARG:CZ	2.35	0.57
2:B:339:TYR:C	2:B:340:GLN:OE1	2.43	0.57
2:B:422:LEU:HB3	2:B:425:LEU:HD12	1.84	0.57
2:B:340:GLN:OE1	2:B:340:GLN:N	2.37	0.57
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.35	0.56
2:B:70:LYS:HG2	2:B:71:TRP:O	2.05	0.56
2:B:157:PRO:HG3	2:B:184:MET:HA	1.88	0.56
1:A:164:MET:HE3	1:A:187:LEU:CD2	2.35	0.56
1:A:369:THR:HG1	1:A:398:TRP:HH2	1.49	0.56
1:A:460:ASN:O	1:A:462:GLY:N	2.34	0.56
2:B:244:ILE:HB	2:B:310:LEU:CD2	2.35	0.56
1:A:2:ILE:HG21	1:A:5:ILE:CG1	2.20	0.56
1:A:10:VAL:HG12	1:A:11:LYS:N	2.20	0.56
1:A:39:THR:HA	4:A:1054:HOH:O	2.05	0.56
1:A:94:ILE:HG13	1:A:229:TRP:CH2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.40	0.56
1:A:219:LYS:O	1:A:221:HIS:N	2.37	0.56
2:B:137:ASN:O	2:B:139:THR:N	2.38	0.56
2:B:278:GLN:HE22	2:B:297:GLU:HB3	1.70	0.56
2:B:298:GLU:HG3	2:B:301:LEU:HD12	1.87	0.56
2:B:369:THR:O	2:B:369:THR:HG22	2.05	0.56
1:A:66:LYS:HB3	1:A:66:LYS:HZ2	1.71	0.56
2:B:100:LEU:O	2:B:100:LEU:HD12	2.05	0.56
2:B:221:HIS:N	2:B:221:HIS:CD2	2.72	0.56
2:B:330:GLN:HE22	2:B:340:GLN:HE22	1.52	0.56
1:A:206:ARG:NH2	1:A:219:LYS:CG	2.69	0.56
1:A:398:TRP:HZ2	1:A:411:ILE:CG2	2.14	0.56
1:A:89:GLU:HB3	1:A:92:LEU:HG	1.88	0.56
1:A:438:GLU:HG3	1:A:460:ASN:ND2	2.16	0.56
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.87	0.56
2:B:362:THR:HG22	2:B:367:GLN:NE2	2.01	0.56
1:A:188:TYR:CE2	3:A:701:ABZ:CL	2.96	0.56
1:A:482:ILE:CD1	1:A:497:THR:HG21	2.35	0.56
1:A:105:SER:OG	1:A:198:HIS:CG	2.59	0.56
1:A:234:LEU:HD13	3:A:701:ABZ:H5	1.88	0.56
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.87	0.56
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.88	0.56
2:B:209:LEU:HB3	2:B:214:LEU:HB2	1.88	0.56
2:B:319:TYR:OH	2:B:385:LYS:HE3	2.05	0.56
1:A:31:ILE:HD12	1:A:133:PRO:O	2.06	0.56
1:A:65:LYS:O	1:A:66:LYS:HB2	2.05	0.56
1:A:220:LYS:O	1:A:220:LYS:HG2	2.04	0.56
1:A:282:LEU:CD2	1:A:296:THR:HG23	2.31	0.56
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.87	0.56
2:B:243:PRO:C	2:B:245:VAL:N	2.57	0.56
2:B:254:VAL:HG21	2:B:288:ALA:O	2.06	0.56
1:A:542:ILE:CG1	1:A:543:GLY:H	2.11	0.55
1:A:451:LYS:HD2	1:A:451:LYS:O	2.06	0.55
2:B:335:GLY:HA2	2:B:367:GLN:OE1	2.06	0.55
1:A:7:THR:HG23	1:A:119:PRO:HB2	1.86	0.55
1:A:126:LYS:HA	1:A:145:GLN:OE1	2.06	0.55
2:B:178:ILE:HD11	2:B:201:LYS:CG	2.36	0.55
2:B:246:LEU:HD21	2:B:310:LEU:HD11	1.89	0.55
2:B:298:GLU:CG	2:B:301:LEU:HB2	2.35	0.55
1:A:398:TRP:CE2	1:A:411:ILE:HG21	2.41	0.55
1:A:460:ASN:HD22	1:A:460:ASN:N	2.02	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASN:C	1:A:462:GLY:H	2.09	0.55
1:A:194:GLU:O	1:A:196:GLY:N	2.40	0.55
2:B:70:LYS:HG3	2:B:71:TRP:H	1.71	0.55
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.66	0.55
1:A:219:LYS:C	1:A:221:HIS:H	2.10	0.55
2:B:146:TYR:CD1	2:B:150:PRO:HB3	2.41	0.55
1:A:515:SER:O	1:A:517:LEU:N	2.40	0.55
2:B:70:LYS:CG	2:B:71:TRP:N	2.70	0.55
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.41	0.55
2:B:246:LEU:HD21	2:B:310:LEU:CD1	2.36	0.55
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.89	0.54
1:A:492:GLU:OE1	1:A:530:LYS:HD2	2.07	0.54
2:B:422:LEU:HB3	2:B:425:LEU:CG	2.37	0.54
1:A:440:PHE:HA	1:A:459:THR:HG22	1.88	0.54
1:A:311:LYS:HE2	1:A:311:LYS:C	2.27	0.54
1:A:334:GLN:HB2	1:A:336:GLN:HE21	1.71	0.54
1:A:460:ASN:ND2	1:A:460:ASN:N	2.56	0.54
2:B:274:ILE:HG21	2:B:306:ASN:HB3	1.88	0.54
1:A:373:GLN:HG2	2:B:394:GLN:NE2	2.22	0.54
2:B:419:THR:N	2:B:420:PRO:HD3	2.23	0.54
1:A:31:ILE:O	1:A:132:ILE:HD11	2.07	0.54
1:A:500:GLN:O	1:A:503:LEU:HB3	2.07	0.54
1:A:513:SER:C	1:A:515:SER:H	2.11	0.54
2:B:173:LYS:O	2:B:176:PRO:HD3	2.06	0.54
1:A:101:LYS:HD3	1:A:103:LYS:NZ	2.22	0.54
1:A:177:ASP:OD1	1:A:177:ASP:N	2.39	0.54
1:A:206:ARG:NH2	1:A:219:LYS:HA	2.22	0.54
2:B:85:GLN:NE2	2:B:89:GLU:HB2	2.23	0.54
2:B:278:GLN:HG3	2:B:299:ALA:CA	2.37	0.54
1:A:301:LEU:O	1:A:304:ALA:HB3	2.08	0.54
2:B:214:LEU:N	2:B:214:LEU:HD23	2.23	0.54
1:A:447:ASN:OD1	1:A:450:THR:HG23	2.07	0.54
1:A:164:MET:O	1:A:167:ILE:N	2.41	0.54
2:B:253:THR:HG22	2:B:292:VAL:CG2	2.30	0.54
2:B:423:VAL:HG12	2:B:423:VAL:O	2.07	0.54
1:A:362:THR:CG2	1:A:363:ASN:N	2.71	0.53
1:A:362:THR:HG23	1:A:363:ASN:N	2.22	0.53
1:A:442:VAL:CG2	1:A:481:ALA:HB1	2.36	0.53
2:B:217:PRO:C	2:B:219:LYS:H	2.11	0.53
1:A:163:SER:O	1:A:167:ILE:HG13	2.09	0.53
2:B:171:PHE:C	2:B:173:LYS:H	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.39	0.53
2:B:260:LEU:HG	2:B:264:LEU:HD11	1.91	0.53
2:B:314:VAL:HG13	2:B:317:VAL:HG21	1.90	0.53
1:A:2:ILE:CG2	1:A:5:ILE:HG13	2.22	0.53
1:A:32:LYS:HA	1:A:35:VAL:HB	1.90	0.53
1:A:347:LYS:HE3	1:A:347:LYS:HA	1.89	0.53
1:A:406:TRP:CH2	2:B:420:PRO:CD	2.91	0.53
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.90	0.53
2:B:243:PRO:O	2:B:245:VAL:HG12	2.09	0.53
1:A:288:ALA:CB	1:A:291:GLU:HB2	2.39	0.53
1:A:320:ASP:OD2	1:A:323:LYS:HG3	2.09	0.53
2:B:253:THR:O	2:B:257:ILE:HG22	2.08	0.53
2:B:260:LEU:CD1	2:B:264:LEU:HD11	2.38	0.53
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.44	0.53
1:A:162:SER:HB2	2:B:52:PRO:CG	2.39	0.53
1:A:229:TRP:CE3	3:A:701:ABZ:H4	2.44	0.53
1:A:479:LEU:HB3	1:A:521:ILE:CD1	2.39	0.53
2:B:90:VAL:O	2:B:92:LEU:N	2.42	0.53
2:B:314:VAL:CG2	2:B:315:HIS:N	2.71	0.53
1:A:17:ASP:CG	1:A:18:GLY:H	2.11	0.53
1:A:206:ARG:NE	1:A:219:LYS:HA	2.23	0.53
1:A:394:GLN:O	1:A:395:LYS:C	2.47	0.53
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.44	0.53
2:B:254:VAL:HG23	2:B:291:GLU:O	2.08	0.53
1:A:54:ASN:C	1:A:56:TYR:H	2.12	0.52
1:A:340:GLN:HB2	1:A:348:ASN:ND2	2.24	0.52
2:B:27:THR:HG22	2:B:29:GLU:N	2.23	0.52
2:B:271:TYR:C	2:B:273:GLY:H	2.11	0.52
2:B:315:HIS:C	2:B:317:VAL:H	2.10	0.52
1:A:298:GLU:H	1:A:298:GLU:CD	2.13	0.52
1:A:330:GLN:OE1	1:A:340:GLN:NE2	2.37	0.52
1:A:393:ILE:O	1:A:416:PHE:HD1	1.92	0.52
1:A:398:TRP:CZ2	1:A:411:ILE:HG21	2.44	0.52
2:B:29:GLU:O	2:B:32:LYS:HB2	2.09	0.52
2:B:263:LYS:HE3	2:B:425:LEU:HB3	1.92	0.52
1:A:394:GLN:O	1:A:397:THR:N	2.40	0.52
2:B:100:LEU:HD11	2:B:106:VAL:HG13	1.91	0.52
1:A:373:GLN:HG2	2:B:394:GLN:HE21	1.73	0.52
2:B:137:ASN:C	2:B:139:THR:N	2.62	0.52
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.39	0.52
2:B:168:LEU:HD21	2:B:209:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LYS:HA	2:B:337:TRP:CE3	2.45	0.52
1:A:2:ILE:HG22	1:A:4:PRO:HG2	1.87	0.52
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.90	0.52
1:A:84:THR:HG21	1:A:153:TRP:NE1	2.22	0.52
1:A:244:ILE:CD1	1:A:310:LEU:HD13	2.40	0.52
1:A:369:THR:OG1	1:A:398:TRP:CH2	2.63	0.52
1:A:406:TRP:CZ3	2:B:420:PRO:CG	2.92	0.52
2:B:131:THR:HG1	2:B:143:ARG:NH1	2.08	0.52
2:B:27:THR:O	2:B:31:ILE:HD12	2.10	0.51
2:B:426:TRP:O	2:B:426:TRP:CD1	2.63	0.51
1:A:12:LEU:HD11	1:A:127:TYR:CE2	2.46	0.51
1:A:65:LYS:HG3	1:A:67:ASP:HB2	1.93	0.51
1:A:134:SER:O	1:A:135:ILE:HB	2.10	0.51
2:B:242:GLN:C	2:B:244:ILE:H	2.13	0.51
2:B:329:ILE:CG2	2:B:330:GLN:N	2.73	0.51
1:A:96:HIS:CE1	1:A:269:GLN:HE21	2.28	0.51
1:A:420:PRO:HA	1:A:421:PRO:O	2.11	0.51
2:B:85:GLN:CB	2:B:154:LYS:HB2	2.40	0.51
2:B:257:ILE:HG23	2:B:258:GLN:N	2.26	0.51
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.75	0.51
2:B:221:HIS:HE1	2:B:230:MET:SD	2.32	0.51
2:B:310:LEU:C	2:B:310:LEU:HD23	2.31	0.51
1:A:125:ARG:O	1:A:128:THR:OG1	2.29	0.51
1:A:491:LEU:HD12	1:A:491:LEU:N	2.20	0.51
2:B:24:TRP:CZ2	2:B:399:GLU:HG2	2.46	0.51
2:B:255:ASN:O	2:B:258:GLN:HB2	2.10	0.51
2:B:274:ILE:HD11	2:B:309:ILE:CG1	2.40	0.51
1:A:2:ILE:HD11	1:A:212:TRP:O	2.11	0.51
1:A:174:GLN:OE1	1:A:175:ASN:ND2	2.40	0.51
1:A:269:GLN:O	1:A:351:THR:N	2.29	0.51
2:B:274:ILE:CD1	2:B:309:ILE:HG12	2.39	0.51
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.25	0.51
1:A:117:SER:HB3	1:A:214:LEU:HD23	1.92	0.51
1:A:167:ILE:O	1:A:170:PRO:HD2	2.10	0.51
1:A:405:TYR:O	2:B:331:LYS:HD3	2.11	0.51
1:A:132:ILE:CG2	1:A:142:ILE:O	2.59	0.51
2:B:422:LEU:HD23	2:B:422:LEU:N	2.24	0.51
1:A:216:THR:C	1:A:218:ASP:N	2.64	0.50
2:B:168:LEU:CD2	2:B:209:LEU:HD21	2.41	0.50
1:A:271:TYR:O	1:A:272:PRO:O	2.29	0.50
1:A:473:THR:HG23	1:A:476:LYS:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:TRP:O	1:A:427:TYR:HB3	2.11	0.50
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.46	0.50
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.41	0.50
1:A:376:THR:O	1:A:380:ILE:HG13	2.11	0.50
1:A:410:TRP:HA	1:A:410:TRP:HE3	1.75	0.50
1:A:215:THR:CG2	1:A:216:THR:N	2.75	0.50
1:A:326:ILE:N	1:A:326:ILE:CD1	2.71	0.50
1:A:417:VAL:HG12	1:A:419:THR:HG22	1.94	0.50
1:A:440:PHE:HE2	1:A:457:TYR:CE2	2.29	0.50
1:A:509:GLN:N	1:A:510:PRO:CD	2.75	0.50
2:B:171:PHE:C	2:B:173:LYS:N	2.64	0.50
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.91	0.50
2:B:128:THR:O	2:B:129:ALA:C	2.49	0.50
2:B:222:GLN:O	2:B:224:GLU:N	2.45	0.50
2:B:249:LYS:NZ	2:B:256:ASP:OD1	2.43	0.50
1:A:17:ASP:CG	1:A:18:GLY:N	2.65	0.50
1:A:101:LYS:HE2	1:A:103:LYS:HZ3	1.77	0.50
1:A:220:LYS:O	1:A:221:HIS:CB	2.60	0.50
1:A:270:ILE:HG13	1:A:314:VAL:HG12	1.93	0.50
1:A:396:GLU:O	1:A:400:THR:HG22	2.12	0.50
2:B:179:VAL:HG23	2:B:179:VAL:O	2.11	0.50
1:A:433:PRO:HB2	1:A:494:ASN:HD21	1.77	0.49
2:B:298:GLU:O	2:B:302:GLU:N	2.34	0.49
2:B:308:GLU:HG2	2:B:309:ILE:H	1.77	0.49
1:A:109:LEU:HB2	1:A:187:LEU:HB3	1.94	0.49
1:A:116:PHE:CZ	1:A:151:GLN:HB2	2.46	0.49
1:A:320:ASP:OD2	1:A:323:LYS:HE3	2.12	0.49
2:B:112:GLY:CA	2:B:185:ASP:HB3	2.43	0.49
1:A:23:GLN:NE2	1:A:131:THR:O	2.45	0.49
1:A:125:ARG:NH2	1:A:147:ASN:HB3	2.27	0.49
1:A:284:ARG:O	1:A:284:ARG:HG2	2.12	0.49
1:A:430:GLU:O	1:A:532:TYR:CD2	2.65	0.49
2:B:155:GLY:O	2:B:159:ILE:HG13	2.11	0.49
2:B:201:LYS:HD3	2:B:204:GLU:OE1	2.12	0.49
2:B:246:LEU:N	2:B:246:LEU:CD2	2.74	0.49
2:B:331:LYS:NZ	2:B:364:ASP:CG	2.65	0.49
1:A:394:GLN:O	1:A:396:GLU:N	2.46	0.49
1:A:479:LEU:HB2	1:A:517:LEU:HD21	1.94	0.49
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.46	0.49
2:B:50:ILE:CG2	2:B:145:GLN:HB3	2.42	0.49
1:A:410:TRP:CD1	2:B:401:TRP:CD2	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HB2	1:A:517:LEU:CD2	2.42	0.49
1:A:66:LYS:HB3	1:A:66:LYS:HZ3	1.76	0.49
1:A:234:LEU:HD13	3:A:701:ABZ:C5	2.42	0.49
1:A:244:ILE:HD11	1:A:310:LEU:CD1	2.40	0.49
1:A:369:THR:CG2	1:A:398:TRP:HH2	2.26	0.49
1:A:502:ALA:O	1:A:506:ILE:HD13	2.12	0.49
1:A:2:ILE:CD1	1:A:212:TRP:O	2.61	0.49
1:A:364:ASP:N	1:A:511:ASP:OD2	2.38	0.49
1:A:439:THR:OG1	2:B:289:LEU:HG	2.12	0.49
2:B:370:GLU:O	2:B:371:ALA:C	2.49	0.49
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.93	0.48
1:A:311:LYS:CA	1:A:311:LYS:HE2	2.41	0.48
1:A:340:GLN:HA	1:A:351:THR:HA	1.93	0.48
1:A:506:ILE:HD12	1:A:506:ILE:N	2.27	0.48
2:B:85:GLN:HG3	2:B:154:LYS:CD	2.43	0.48
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.93	0.48
1:A:204:GLU:O	1:A:205:LEU:C	2.51	0.48
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.96	0.48
2:B:84:THR:C	2:B:86:ASP:N	2.66	0.48
2:B:100:LEU:HD13	2:B:179:VAL:CG2	2.43	0.48
2:B:419:THR:O	2:B:421:PRO:CD	2.60	0.48
2:B:236:PRO:HA	2:B:239:TRP:CG	2.49	0.48
2:B:298:GLU:HG2	2:B:301:LEU:HB2	1.95	0.48
1:A:280:SER:O	1:A:283:LEU:N	2.45	0.48
1:A:362:THR:CG2	1:A:367:GLN:HE21	2.23	0.48
2:B:193:LEU:HB3	2:B:197:GLN:HB2	1.96	0.48
2:B:295:LEU:HD12	2:B:296:THR:O	2.14	0.48
1:A:442:VAL:HG22	1:A:481:ALA:CB	2.40	0.48
2:B:226:PRO:O	2:B:227:PHE:CD2	2.67	0.48
2:B:274:ILE:HD13	2:B:306:ASN:HA	1.95	0.48
2:B:308:GLU:HG3	2:B:309:ILE:N	2.29	0.48
1:A:100:LEU:HA	3:A:701:ABZ:H13	1.96	0.48
2:B:266:TRP:HB3	2:B:426:TRP:CE3	2.49	0.48
2:B:274:ILE:HG12	2:B:309:ILE:HD11	1.95	0.48
1:A:344:GLU:OE1	1:A:344:GLU:CA	2.62	0.48
2:B:265:ASN:O	2:B:268:SER:HB3	2.13	0.48
2:B:324:ASP:O	2:B:343:GLN:HG2	2.13	0.47
2:B:329:ILE:CG2	2:B:330:GLN:H	2.26	0.47
2:B:401:TRP:O	2:B:404:GLU:N	2.44	0.47
1:A:432:GLU:HG3	1:A:433:PRO:HD2	1.96	0.47
1:A:442:VAL:HG12	1:A:496:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ILE:O	2:B:258:GLN:C	2.52	0.47
2:B:266:TRP:C	2:B:268:SER:N	2.65	0.47
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.97	0.47
2:B:70:LYS:CG	2:B:71:TRP:H	2.27	0.47
2:B:115:TYR:N	2:B:115:TYR:CD2	2.81	0.47
1:A:64:LYS:HE3	1:A:68:SER:OG	2.14	0.47
1:A:157:PRO:HD2	4:A:1080:HOH:O	2.14	0.47
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.97	0.47
2:B:266:TRP:CE3	2:B:266:TRP:CA	2.96	0.47
2:B:418:ASN:ND2	2:B:418:ASN:H	2.11	0.47
1:A:54:ASN:ND2	1:A:129:ALA:CB	2.74	0.47
1:A:74:LEU:HD12	1:A:75:VAL:N	2.30	0.47
1:A:173:LYS:C	1:A:175:ASN:H	2.17	0.47
1:A:491:LEU:H	1:A:491:LEU:CD1	2.19	0.47
1:A:504:GLY:O	1:A:505:ILE:C	2.53	0.47
1:A:519:ASN:O	1:A:523:GLU:HG2	2.15	0.47
2:B:87:PHE:C	2:B:88:TRP:HD1	2.18	0.47
2:B:370:GLU:O	2:B:372:VAL:N	2.48	0.47
1:A:130:PHE:CD1	1:A:130:PHE:C	2.88	0.47
1:A:168:LEU:O	1:A:170:PRO:N	2.48	0.47
2:B:254:VAL:O	2:B:257:ILE:HG23	2.14	0.47
1:A:40:GLU:OE2	1:A:43:LYS:HD3	2.15	0.47
1:A:178:ILE:CG2	1:A:189:VAL:HG13	2.44	0.47
1:A:263:LYS:HE2	4:A:1129:HOH:O	2.14	0.47
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.15	0.47
1:A:297:GLU:CD	1:A:297:GLU:H	2.17	0.47
2:B:56:TYR:O	2:B:143:ARG:NH2	2.41	0.47
2:B:134:SER:CB	2:B:139:THR:HG22	2.43	0.47
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.44	0.47
2:B:317:VAL:HG11	2:B:348:ASN:O	2.15	0.47
2:B:354:TYR:CD1	2:B:355:ALA:N	2.82	0.47
2:B:376:THR:O	2:B:377:THR:C	2.53	0.47
2:B:388:LYS:HA	2:B:413:GLU:O	2.14	0.47
2:B:418:ASN:H	2:B:418:ASN:HD22	1.60	0.47
2:B:173:LYS:O	2:B:174:GLN:C	2.54	0.47
1:A:153:TRP:HZ3	1:A:159:ILE:HD12	1.80	0.47
1:A:399:GLU:HG3	1:A:402:TRP:NE1	2.29	0.47
1:A:12:LEU:O	1:A:13:LYS:C	2.53	0.47
1:A:126:LYS:HB3	1:A:126:LYS:HE2	1.55	0.47
1:A:205:LEU:O	1:A:208:HIS:HB3	2.15	0.47
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:LYS:NZ	2:B:116:PHE:CD1	2.77	0.47
1:A:410:TRP:HD1	2:B:401:TRP:CE2	2.33	0.46
2:B:288:ALA:HB3	2:B:291:GLU:HB2	1.98	0.46
2:B:422:LEU:C	2:B:424:LYS:H	2.16	0.46
1:A:326:ILE:HG22	1:A:327:ALA:N	2.31	0.46
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.50	0.46
1:A:427:TYR:OH	1:A:509:GLN:HA	2.15	0.46
2:B:277:ARG:O	2:B:281:LYS:HB3	2.14	0.46
2:B:419:THR:H	2:B:420:PRO:CD	2.26	0.46
1:A:101:LYS:HE3	1:A:321:PRO:CG	2.45	0.46
1:A:188:TYR:CD2	3:A:701:ABZ:CL	3.05	0.46
1:A:215:THR:HG22	1:A:216:THR:H	1.79	0.46
1:A:233:GLU:HB3	1:A:240:THR:HG22	1.96	0.46
1:A:398:TRP:NE1	1:A:402:TRP:HD1	2.14	0.46
1:A:481:ALA:O	1:A:482:ILE:C	2.52	0.46
2:B:44:GLU:OE1	2:B:46:LYS:HE3	2.15	0.46
1:A:153:TRP:CZ3	1:A:159:ILE:HD12	2.51	0.46
1:A:244:ILE:CD1	1:A:310:LEU:HD22	2.37	0.46
2:B:266:TRP:CZ3	2:B:269:GLN:CB	2.98	0.46
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.97	0.46
2:B:73:LYS:HE2	2:B:75:VAL:CG2	2.45	0.46
2:B:367:GLN:O	2:B:370:GLU:HB2	2.15	0.46
1:A:465:LYS:HE2	1:A:488:ASP:OD2	2.16	0.46
2:B:84:THR:C	2:B:86:ASP:H	2.17	0.46
2:B:90:VAL:C	2:B:92:LEU:H	2.19	0.46
2:B:276:VAL:O	2:B:279:LEU:N	2.45	0.46
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.51	0.46
1:A:46:LYS:HD3	1:A:116:PHE:HB3	1.98	0.46
1:A:162:SER:HB2	2:B:52:PRO:HG2	1.97	0.46
1:A:493:VAL:HG22	1:A:494:ASN:N	2.31	0.46
1:A:509:GLN:N	1:A:510:PRO:HD3	2.30	0.46
2:B:281:LYS:C	2:B:283:LEU:H	2.19	0.46
2:B:339:TYR:CG	2:B:375:ILE:HD13	2.51	0.46
2:B:419:THR:O	2:B:419:THR:HG22	2.16	0.46
1:A:101:LYS:CD	1:A:103:LYS:NZ	2.78	0.46
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.51	0.46
2:B:349:LEU:HD23	2:B:349:LEU:HA	1.68	0.46
1:A:363:ASN:OD1	1:A:365:VAL:N	2.50	0.45
1:A:469:LEU:CD1	1:A:477:THR:HG22	2.46	0.45
2:B:100:LEU:HD13	2:B:179:VAL:HG23	1.98	0.45
1:A:242:GLN:O	1:A:243:PRO:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ASP:CB	1:A:326:ILE:HD11	2.44	0.45
1:A:362:THR:HG21	1:A:367:GLN:CG	2.40	0.45
2:B:66:LYS:C	2:B:68:SER:H	2.18	0.45
1:A:298:GLU:CD	1:A:298:GLU:N	2.69	0.45
1:A:407:GLN:OE1	2:B:394:GLN:N	2.49	0.45
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.28	0.45
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.50	0.45
1:A:509:GLN:O	1:A:510:PRO:C	2.55	0.45
2:B:320:ASP:OD1	2:B:322:SER:OG	2.34	0.45
1:A:85:GLN:C	1:A:154:LYS:HZ3	2.18	0.45
2:B:203:GLU:HA	2:B:206:ARG:CB	2.43	0.45
1:A:98:ALA:HB2	1:A:350:LYS:HB2	1.98	0.45
1:A:265:ASN:O	1:A:268:SER:HB3	2.17	0.45
1:A:478:GLU:OE2	1:A:499:SER:HB2	2.16	0.45
2:B:353:LYS:HG2	2:B:354:TYR:N	2.31	0.45
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.52	0.45
1:A:116:PHE:HD2	1:A:148:VAL:HG21	1.81	0.45
1:A:350:LYS:HG2	1:A:351:THR:N	2.31	0.45
2:B:230:MET:HE3	4:B:1037:HOH:O	2.16	0.45
1:A:95:PRO:HG2	1:A:229:TRP:CH2	2.52	0.45
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.51	0.45
1:A:280:SER:C	1:A:282:LEU:N	2.69	0.45
1:A:478:GLU:OE2	1:A:499:SER:HB3	2.16	0.45
2:B:125:ARG:HD3	2:B:146:TYR:O	2.17	0.45
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.16	0.45
1:A:20:LYS:CE	1:A:55:PRO:HB2	2.44	0.45
1:A:23:GLN:OE1	1:A:60:VAL:O	2.35	0.45
1:A:101:LYS:HG2	1:A:103:LYS:HE2	1.99	0.45
1:A:473:THR:O	1:A:476:LYS:N	2.49	0.45
1:A:142:ILE:H	1:A:142:ILE:HG13	1.57	0.45
2:B:339:TYR:O	2:B:339:TYR:CD2	2.70	0.44
2:B:354:TYR:CG	2:B:355:ALA:N	2.85	0.44
2:B:389:PHE:HB3	2:B:391:LEU:CD2	2.47	0.44
1:A:246:LEU:HD13	1:A:303:LEU:HD11	1.99	0.44
1:A:406:TRP:CE2	2:B:420:PRO:HD2	2.51	0.44
2:B:52:PRO:C	2:B:54:ASN:H	2.20	0.44
2:B:60:VAL:O	2:B:60:VAL:HG23	2.16	0.44
2:B:222:GLN:C	2:B:224:GLU:H	2.19	0.44
1:A:164:MET:HE3	1:A:187:LEU:CD1	2.47	0.44
1:A:407:GLN:CG	2:B:393:ILE:HA	2.48	0.44
2:B:306:ASN:C	2:B:308:GLU:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.16	0.44
1:A:101:LYS:HE3	1:A:321:PRO:HG3	1.99	0.44
1:A:212:TRP:C	1:A:214:LEU:H	2.20	0.44
1:A:525:LEU:HD23	1:A:525:LEU:HA	1.84	0.44
2:B:240:THR:CG2	2:B:241:VAL:N	2.78	0.44
2:B:278:GLN:HG3	2:B:299:ALA:N	2.32	0.44
2:B:278:GLN:CG	2:B:299:ALA:N	2.81	0.44
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.53	0.44
1:A:183:TYR:O	1:A:186:ASP:N	2.48	0.44
1:A:369:THR:OG1	1:A:398:TRP:HH2	1.99	0.44
1:A:442:VAL:HG21	1:A:482:ILE:HA	1.99	0.44
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.52	0.44
2:B:129:ALA:HA	2:B:144:TYR:O	2.17	0.44
2:B:339:TYR:OH	2:B:378:GLU:OE1	2.34	0.44
1:A:442:VAL:HG21	1:A:482:ILE:N	2.33	0.44
2:B:239:TRP:O	2:B:240:THR:OG1	2.30	0.44
2:B:257:ILE:HG13	2:B:261:VAL:HG23	2.00	0.44
1:A:116:PHE:HD2	1:A:148:VAL:CG2	2.31	0.44
1:A:416:PHE:HE2	1:A:418:ASN:HB2	1.82	0.44
1:A:28:GLU:CA	1:A:31:ILE:HG22	2.46	0.43
1:A:221:HIS:O	1:A:222:GLN:C	2.56	0.43
2:B:330:GLN:HE22	2:B:340:GLN:NE2	2.15	0.43
2:B:379:SER:HA	2:B:383:TRP:CZ3	2.53	0.43
1:A:483:TYR:HB2	1:A:521:ILE:CG1	2.48	0.43
2:B:169:GLU:N	2:B:170:PRO:HD2	2.33	0.43
1:A:2:ILE:HG23	1:A:4:PRO:CG	2.35	0.43
1:A:116:PHE:CD2	1:A:148:VAL:HG21	2.53	0.43
1:A:233:GLU:OE1	1:A:235:HIS:NE2	2.48	0.43
1:A:295:LEU:HB3	1:A:300:GLU:HG2	2.01	0.43
1:A:513:SER:O	1:A:519:ASN:ND2	2.51	0.43
3:A:701:ABZ:H13	2:B:138:GLU:CD	2.39	0.43
2:B:194:GLU:O	2:B:195:ILE:C	2.55	0.43
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.54	0.43
2:B:260:LEU:HD11	2:B:264:LEU:HD11	2.00	0.43
2:B:306:ASN:C	2:B:308:GLU:N	2.72	0.43
1:A:216:THR:C	1:A:218:ASP:H	2.19	0.43
2:B:64:LYS:HD2	2:B:71:TRP:CE3	2.53	0.43
2:B:330:GLN:HG2	2:B:338:THR:O	2.19	0.43
1:A:513:SER:C	1:A:515:SER:N	2.71	0.43
2:B:172:LYS:HE2	2:B:172:LYS:HB3	1.81	0.43
1:A:115:TYR:O	1:A:149:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PHE:CE2	1:A:153:TRP:HZ2	2.36	0.43
2:B:265:ASN:O	2:B:268:SER:CB	2.67	0.43
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.85	0.43
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	3.07	0.43
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.51	0.43
2:B:3:SER:N	2:B:4:PRO:CD	2.78	0.43
2:B:298:GLU:HG3	2:B:301:LEU:HB2	2.01	0.43
1:A:18:GLY:HA3	1:A:127:TYR:HD2	1.83	0.43
1:A:405:TYR:O	2:B:331:LYS:CD	2.67	0.43
2:B:221:HIS:CE1	2:B:230:MET:SD	3.11	0.43
1:A:10:VAL:CG1	1:A:11:LYS:N	2.82	0.43
1:A:30:LYS:HA	1:A:33:ALA:CB	2.47	0.43
1:A:540:LYS:HD2	2:B:265:ASN:HD22	1.82	0.43
2:B:90:VAL:C	2:B:92:LEU:N	2.73	0.43
1:A:64:LYS:HA	1:A:64:LYS:HD3	1.80	0.43
1:A:107:THR:HB	1:A:221:HIS:HB3	2.01	0.43
1:A:332:GLN:HB2	1:A:336:GLN:HB2	2.00	0.43
1:A:457:TYR:CZ	1:A:465:LYS:HB3	2.53	0.43
1:A:34:LEU:O	1:A:38:CYS:N	2.48	0.42
1:A:397:THR:O	1:A:400:THR:CG2	2.67	0.42
1:A:470:THR:O	1:A:471:ASN:CB	2.58	0.42
1:A:1:PRO:C	1:A:2:ILE:CG1	2.88	0.42
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.55	0.42
1:A:486:LEU:CD2	1:A:495:ILE:HD11	2.47	0.42
2:B:168:LEU:HD13	2:B:180:ILE:HD12	2.00	0.42
2:B:379:SER:CB	2:B:387:PRO:HD3	2.49	0.42
1:A:155:GLY:O	1:A:159:ILE:HG13	2.19	0.42
1:A:496:VAL:O	1:A:496:VAL:HG12	2.18	0.42
1:A:23:GLN:CD	1:A:60:VAL:H	2.22	0.42
1:A:125:ARG:NE	1:A:147:ASN:HA	2.32	0.42
1:A:217:PRO:HA	1:A:219:LYS:HZ3	1.83	0.42
1:A:341:ILE:HD11	1:A:375:ILE:HG23	2.00	0.42
2:B:421:PRO:C	2:B:423:VAL:N	2.66	0.42
1:A:101:LYS:HE3	1:A:321:PRO:CD	2.50	0.42
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.55	0.42
1:A:174:GLN:O	1:A:175:ASN:CG	2.58	0.42
1:A:246:LEU:CD1	1:A:310:LEU:HD12	2.45	0.42
1:A:440:PHE:CD2	1:A:459:THR:CG2	3.03	0.42
1:A:483:TYR:HB2	1:A:521:ILE:HG12	2.00	0.42
2:B:136:ASN:O	2:B:138:GLU:N	2.53	0.42
2:B:241:VAL:HG22	2:B:243:PRO:CD	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:HB2	2:B:336:GLN:C	2.39	0.42
1:A:481:ALA:O	1:A:484:LEU:HB3	2.20	0.42
2:B:364:ASP:O	2:B:367:GLN:HB2	2.19	0.42
1:A:173:LYS:HB3	1:A:173:LYS:HE2	1.83	0.42
2:B:230:MET:O	2:B:231:GLY:C	2.58	0.42
2:B:303:LEU:HA	2:B:306:ASN:HD22	1.81	0.42
2:B:350:LYS:O	2:B:350:LYS:HG2	2.19	0.42
2:B:370:GLU:C	2:B:372:VAL:N	2.72	0.42
2:B:388:LYS:HE2	4:B:1097:HOH:O	2.20	0.42
1:A:235:HIS:CD2	1:A:235:HIS:N	2.87	0.42
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.80	0.42
2:B:244:ILE:HD13	2:B:271:TYR:OH	2.19	0.42
2:B:298:GLU:HG3	2:B:301:LEU:HD13	2.00	0.42
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.26	0.42
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.85	0.42
1:A:482:ILE:O	1:A:485:ALA:HB3	2.19	0.42
2:B:43:LYS:C	2:B:45:GLY:N	2.71	0.42
2:B:376:THR:HG21	2:B:410:TRP:CH2	2.55	0.42
1:A:91:GLN:O	1:A:91:GLN:CG	2.65	0.41
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.55	0.41
2:B:103:LYS:HD2	2:B:191:SER:CA	2.51	0.41
2:B:131:THR:HA	2:B:142:ILE:O	2.20	0.41
2:B:140:PRO:O	2:B:141:GLY:C	2.56	0.41
2:B:303:LEU:CD2	2:B:307:ARG:NH1	2.78	0.41
2:B:339:TYR:CG	2:B:375:ILE:CD1	3.03	0.41
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.50	0.41
1:A:2:ILE:HD13	1:A:5:ILE:HG13	2.02	0.41
2:B:411:ILE:O	2:B:412:PRO:C	2.54	0.41
1:A:108:VAL:CG2	1:A:109:LEU:N	2.81	0.41
1:A:116:PHE:O	1:A:148:VAL:HG11	2.19	0.41
1:A:137:ASN:O	1:A:137:ASN:CG	2.58	0.41
1:A:189:VAL:HG21	1:A:205:LEU:HD22	2.02	0.41
1:A:183:TYR:CD2	1:A:229:TRP:NE1	2.87	0.41
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.36	0.41
1:A:111:VAL:HG23	1:A:185:ASP:O	2.20	0.41
1:A:162:SER:CB	2:B:52:PRO:HG2	2.51	0.41
1:A:229:TRP:CZ3	3:A:701:ABZ:H4	2.55	0.41
1:A:325:LEU:C	1:A:326:ILE:HD12	2.40	0.41
2:B:260:LEU:CG	2:B:264:LEU:HD11	2.49	0.41
2:B:300:GLU:OE1	2:B:303:LEU:HD23	2.20	0.41
2:B:342:TYR:CD1	2:B:342:TYR:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:ILE:C	2:B:412:PRO:O	2.59	0.41
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.51	0.41
1:A:168:LEU:O	1:A:169:GLU:C	2.58	0.41
1:A:379:SER:HA	1:A:383:TRP:CE3	2.55	0.41
1:A:432:GLU:O	1:A:433:PRO:O	2.38	0.41
2:B:85:GLN:HE21	2:B:89:GLU:HB2	1.85	0.41
2:B:325:LEU:HD12	2:B:385:LYS:HG3	2.03	0.41
2:B:392:PRO:O	2:B:392:PRO:HG2	2.21	0.41
1:A:30:LYS:O	1:A:33:ALA:HB3	2.20	0.41
1:A:101:LYS:HB2	3:A:701:ABZ:N6	2.35	0.41
2:B:43:LYS:C	2:B:45:GLY:H	2.24	0.41
2:B:103:LYS:HD2	2:B:191:SER:HA	2.02	0.41
1:A:50:ILE:HD12	1:A:145:GLN:OE1	2.21	0.41
1:A:110:ASP:HB3	1:A:218:ASP:OD2	2.20	0.41
1:A:253:THR:HG22	1:A:256:ASP:CG	2.41	0.41
1:A:270:ILE:HG23	1:A:271:TYR:CD1	2.55	0.41
2:B:160:PHE:O	2:B:161:GLN:C	2.59	0.41
2:B:310:LEU:O	2:B:310:LEU:HD23	2.21	0.41
2:B:369:THR:O	2:B:369:THR:CG2	2.68	0.41
1:A:1:PRO:CD	1:A:117:SER:HA	2.51	0.41
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.56	0.41
2:B:230:MET:O	2:B:231:GLY:O	2.39	0.41
2:B:259:LYS:O	2:B:260:LEU:C	2.59	0.41
2:B:271:TYR:C	2:B:273:GLY:N	2.74	0.41
2:B:411:ILE:O	2:B:412:PRO:O	2.38	0.41
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.82	0.41
1:A:484:LEU:O	1:A:487:GLN:HB2	2.21	0.41
2:B:140:PRO:O	2:B:141:GLY:O	2.38	0.41
2:B:241:VAL:HG11	2:B:351:THR:OG1	2.20	0.41
2:B:266:TRP:C	2:B:268:SER:H	2.23	0.41
2:B:278:GLN:NE2	2:B:297:GLU:HB3	2.34	0.41
2:B:340:GLN:NE2	2:B:427:TYR:CE1	2.89	0.41
1:A:412:PRO:O	1:A:414:TRP:HD1	2.04	0.40
2:B:34:LEU:HD21	2:B:61:PHE:O	2.20	0.40
2:B:78:ARG:HD3	2:B:412:PRO:O	2.21	0.40
1:A:50:ILE:CD1	1:A:54:ASN:HD22	2.18	0.40
1:A:357:MET:O	1:A:358:ARG:C	2.60	0.40
2:B:47:ILE:HD12	2:B:130:PHE:HZ	1.86	0.40
2:B:265:ASN:O	2:B:265:ASN:OD1	2.39	0.40
2:B:276:VAL:O	2:B:277:ARG:C	2.59	0.40
1:A:164:MET:CE	1:A:187:LEU:HD22	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CD2	2:B:420:PRO:HG2	2.51	0.40
2:B:87:PHE:O	2:B:88:TRP:HD1	2.04	0.40
2:B:90:VAL:HG12	2:B:91:GLN:N	2.36	0.40
2:B:125:ARG:O	2:B:126:LYS:C	2.59	0.40
1:A:34:LEU:HB2	1:A:132:ILE:CD1	2.52	0.40
1:A:275:LYS:O	1:A:276:VAL:CG2	2.69	0.40
1:A:433:PRO:CB	1:A:494:ASN:HD21	2.34	0.40
2:B:325:LEU:HD23	2:B:325:LEU:HA	1.84	0.40
1:A:117:SER:CB	1:A:214:LEU:HD23	2.52	0.40
1:A:217:PRO:O	1:A:219:LYS:CD	2.69	0.40
1:A:447:ASN:CG	1:A:450:THR:HG23	2.41	0.40
1:A:519:ASN:O	1:A:523:GLU:CG	2.69	0.40
2:B:5:ILE:HG22	2:B:6:GLU:N	2.37	0.40
2:B:244:ILE:H	2:B:244:ILE:HG13	1.53	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	541/560 (97%)	415 (77%)	89 (16%)	37 (7%)	1 3
2	B	423/430 (98%)	323 (76%)	68 (16%)	32 (8%)	1 2
All	All	964/990 (97%)	738 (77%)	157 (16%)	69 (7%)	1 2

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	55	PRO
1	A	113	ASP
1	A	141	GLY

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Mol	Chain	Res	Type
1	A	151	GLN
1	A	220	LYS
1	A	222	GLN
1	A	272	PRO
1	A	287	LYS
1	A	461	LYS
1	A	516	GLU
1	A	538	ALA
1	A	539	HIS
2	B	65	LYS
2	B	67	ASP
2	B	85	GLN
2	B	137	ASN
2	B	223	LYS
2	B	297	GLU
1	A	112	GLY
1	A	169	GLU
1	A	195	ILE
1	A	219	LYS
1	A	273	GLY
1	A	276	VAL
1	A	395	LYS
1	A	471	ASN
1	A	541	GLY
2	B	91	GLN
2	B	116	PHE
2	B	218	ASP
2	B	231	GLY
2	B	241	VAL
2	B	294	PRO
2	B	376	THR
2	B	377	THR
1	A	170	PRO
1	A	221	HIS
1	A	243	PRO
1	A	358	ARG
1	A	433	PRO
1	A	503	LEU
1	A	513	SER
2	B	68	SER
2	B	141	GLY
2	B	232	TYR

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Mol	Chain	Res	Type
2	B	419	THR
2	B	422	LEU
1	A	52	PRO
1	A	412	PRO
1	A	427	TYR
2	B	138	GLU
2	B	350	LYS
2	B	420	PRO
1	A	213	GLY
1	A	283	LEU
2	B	126	LYS
2	B	162	SER
2	B	242	GLN
2	B	335	GLY
1	A	420	PRO
1	A	135	ILE
2	B	244	ILE
2	B	412	PRO
1	A	387	PRO
2	B	150	PRO
2	B	195	ILE
2	B	112	GLY
2	B	243	PRO

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	486/500 (97%)	444 (91%)	42 (9%)	10 30
2	B	387/392 (99%)	354 (92%)	33 (8%)	10 31
All	All	873/892 (98%)	798 (91%)	75 (9%)	10 30

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

Mol	Chain	Res	Type
1	A	3	SER
1	A	23	GLN
1	A	31	ILE
1	A	32	LYS
1	A	67	ASP
1	A	70	LYS
1	A	71	TRP
1	A	94	ILE
1	A	111	VAL
1	A	137	ASN
1	A	139	THR
1	A	156	SER
1	A	162	SER
1	A	164	MET
1	A	177	ASP
1	A	201	LYS
1	A	251	SER
1	A	286	THR
1	A	287	LYS
1	A	295	LEU
1	A	311	LYS
1	A	330	GLN
1	A	347	LYS
1	A	362	THR
1	A	363	ASN
1	A	369	THR
1	A	387	PRO
1	A	394	GLN
1	A	402	TRP
1	A	410	TRP
1	A	413	GLU
1	A	418	ASN
1	A	431	LYS
1	A	451	LYS
1	A	460	ASN
1	A	491	LEU
1	A	496	VAL
1	A	497	THR
1	A	510	PRO
1	A	514	GLU
1	A	523	GLU
1	A	529	GLU
2	B	12	LEU

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Mol	Chain	Res	Type
2	B	40	GLU
2	B	67	ASP
2	B	72	ARG
2	B	91	GLN
2	B	109	LEU
2	B	139	THR
2	B	150	PRO
2	B	206	ARG
2	B	221	HIS
2	B	232	TYR
2	B	239	TRP
2	B	242	GLN
2	B	244	ILE
2	B	246	LEU
2	B	266	TRP
2	B	274	ILE
2	B	277	ARG
2	B	294	PRO
2	B	302	GLU
2	B	305	GLU
2	B	309	ILE
2	B	310	LEU
2	B	330	GLN
2	B	340	GLN
2	B	357	MET
2	B	363	ASN
2	B	374	LYS
2	B	399	GLU
2	B	400	THR
2	B	410	TRP
2	B	418	ASN
2	B	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	96	HIS
1	A	137	ASN
1	A	269	GLN
1	A	278	GLN
1	A	460	ASN

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Mol	Chain	Res	Type
1	A	475	GLN
1	A	494	ASN
1	A	509	GLN
1	A	519	ASN
2	B	136	ASN
2	B	174	GLN
2	B	207	GLN
2	B	208	HIS
2	B	221	HIS
2	B	258	GLN
2	B	278	GLN
2	B	330	GLN
2	B	336	GLN
2	B	363	ASN
2	B	367	GLN
2	B	407	GLN
2	B	418	ASN

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 monosaccharides 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	ABZ	A	701	-	28,30,30	1.88	9 (32%)	37,42,42	2.45	14 (37%)

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	ABZ	A	701	-	-	4/10/10/10	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ABZ	C10-N4	4.34	1.42	1.33
3	A	701	ABZ	C16-C11	3.44	1.45	1.39
3	A	701	ABZ	C8-N3	3.13	1.38	1.33
3	A	701	ABZ	C16-C15	2.95	1.44	1.38
3	A	701	ABZ	C10-N2	2.37	1.39	1.35
3	A	701	ABZ	C13-C14	2.30	1.44	1.39
3	A	701	ABZ	C13-C12	2.20	1.42	1.38
3	A	701	ABZ	C12-C11	2.18	1.42	1.39
3	A	701	ABZ	C4-C5	2.17	1.41	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ABZ	C10-N3-C8	6.45	118.58	114.19
3	A	701	ABZ	C7-C1-C2	5.71	127.98	121.70
3	A	701	ABZ	C9-N1-C8	4.11	120.24	114.47
3	A	701	ABZ	N3-C10-N2	-4.04	119.08	125.42
3	A	701	ABZ	N2-C9-N1	-3.99	119.92	126.23
3	A	701	ABZ	C5-C4-C3	-3.92	115.91	120.84
3	A	701	ABZ	C10-N2-C9	3.73	120.06	113.75
3	A	701	ABZ	C11-N5-C9	-3.41	119.33	129.23
3	A	701	ABZ	C7-C1-C6	-3.39	117.22	121.88
3	A	701	ABZ	N3-C8-N1	-3.02	122.08	126.06
3	A	701	ABZ	C25-C2-C3	-2.76	103.83	106.18
3	A	701	ABZ	N4-C10-N2	2.59	121.28	117.25
3	A	701	ABZ	C4-C5-C6	2.53	121.98	119.63
3	A	701	ABZ	C7-C8-N3	2.11	120.86	117.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

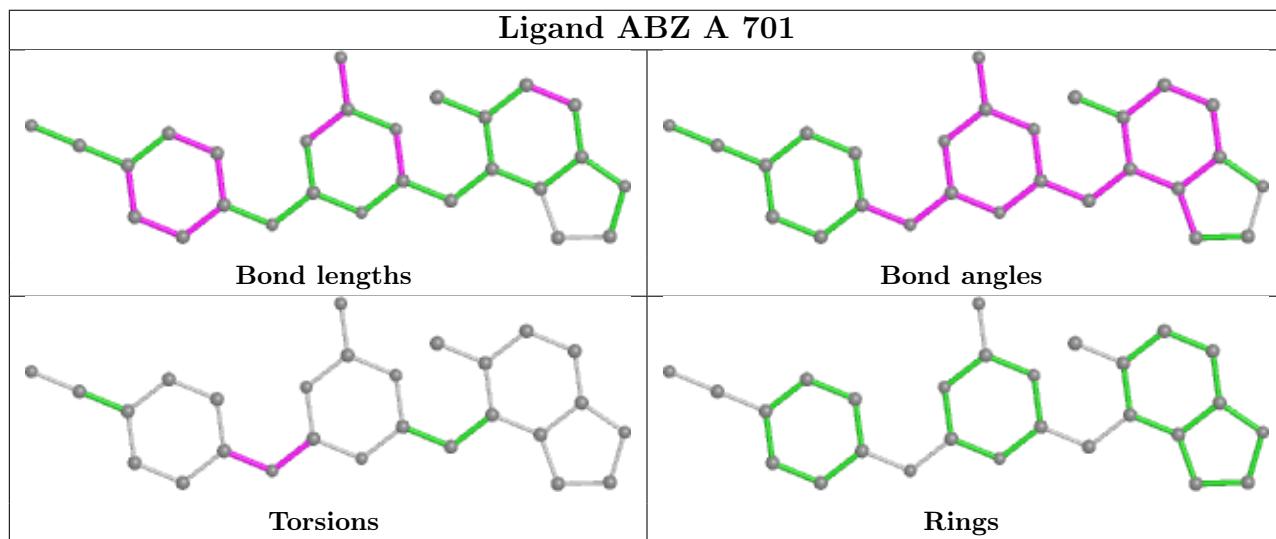
Mol	Chain	Res	Type	Atoms
3	A	701	ABZ	N1-C9-N5-C11
3	A	701	ABZ	N2-C9-N5-C11
3	A	701	ABZ	C16-C11-N5-C9
3	A	701	ABZ	C12-C11-N5-C9

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	ABZ	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/560 (96%)	-0.17	15 (2%) 53 43	29, 78, 110, 112	17 (3%)
2	B	425/430 (98%)	-0.08	21 (4%) 29 20	16, 63, 111, 112	14 (3%)
All	All	968/990 (97%)	-0.13	36 (3%) 41 31	16, 75, 111, 112	31 (3%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	SER	5.4
2	B	229	TRP	5.0
2	B	225	PRO	4.1
1	A	140	PRO	4.1
1	A	2	ILE	3.8
2	B	226	PRO	3.7
2	B	230	MET	3.6
2	B	360	ALA	3.5
2	B	224	GLU	3.5
2	B	227	PHE	3.4
1	A	357	MET	3.4
1	A	65	LYS	3.2
1	A	360	ALA	3.1
2	B	222	GLN	3.1
2	B	4	PRO	3.0
1	A	217	PRO	2.9
2	B	223	LYS	2.9
2	B	228	LEU	2.9
2	B	284	ARG	2.8
2	B	220	LYS	2.7
2	B	358	ARG	2.6
1	A	68	SER	2.6
2	B	218	ASP	2.4
1	A	101	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	359	GLY	2.4
1	A	133	PRO	2.4
2	B	315	HIS	2.3
2	B	15	GLY	2.3
1	A	136	ASN	2.2
2	B	311	LYS	2.2
2	B	359	GLY	2.1
1	A	67	ASP	2.1
2	B	357	MET	2.1
1	A	358	ARG	2.0
1	A	66	LYS	2.0
1	A	3	SER	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 [\(i\)](#)

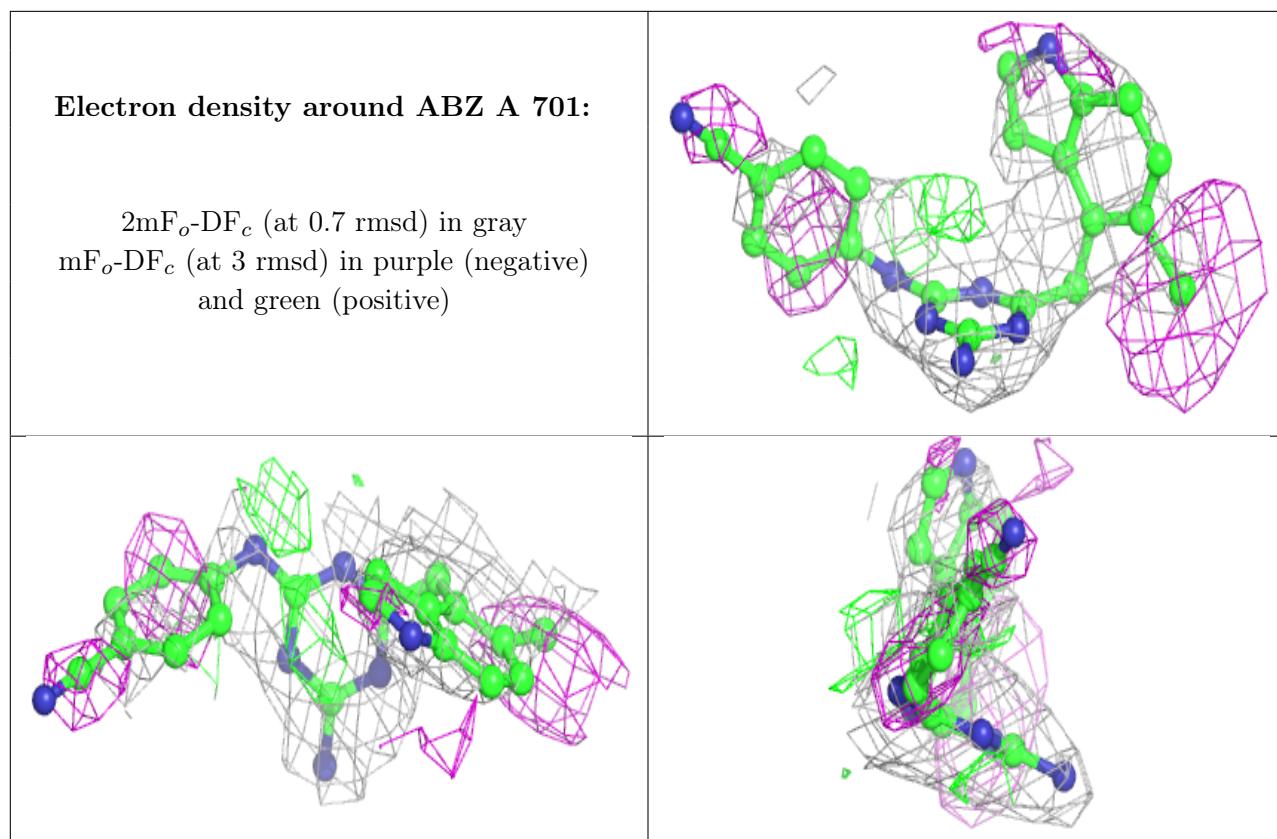
There are no monosaccharides in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ABZ	A	701	27/27	0.75	0.34	43,63,70,73	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.