



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:54 PM UTC

PDB ID : 1S9G / pdb_00001s9g
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

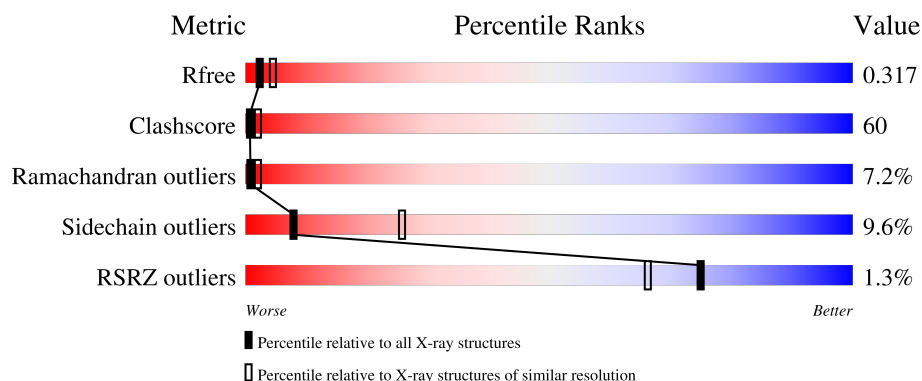
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	
2	B	430	

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

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
1	A	543	Total	C	N	O	S	66	0	0
			4429	2871	736	815	7			

There is a discrepancy between the modelled and reference sequences:

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

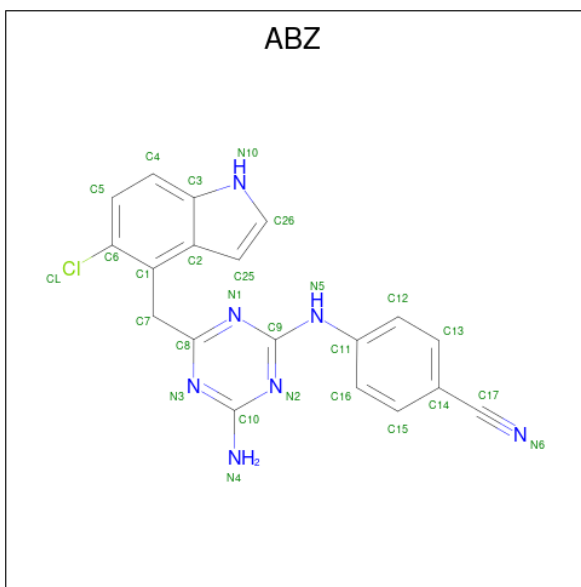
- Molecule 2 is a protein called POL polyprotein [Contains: Reverse transcriptase].

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

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 (CCD ID: ABZ) (formula: C₁₉H₁₄ClN₇).



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

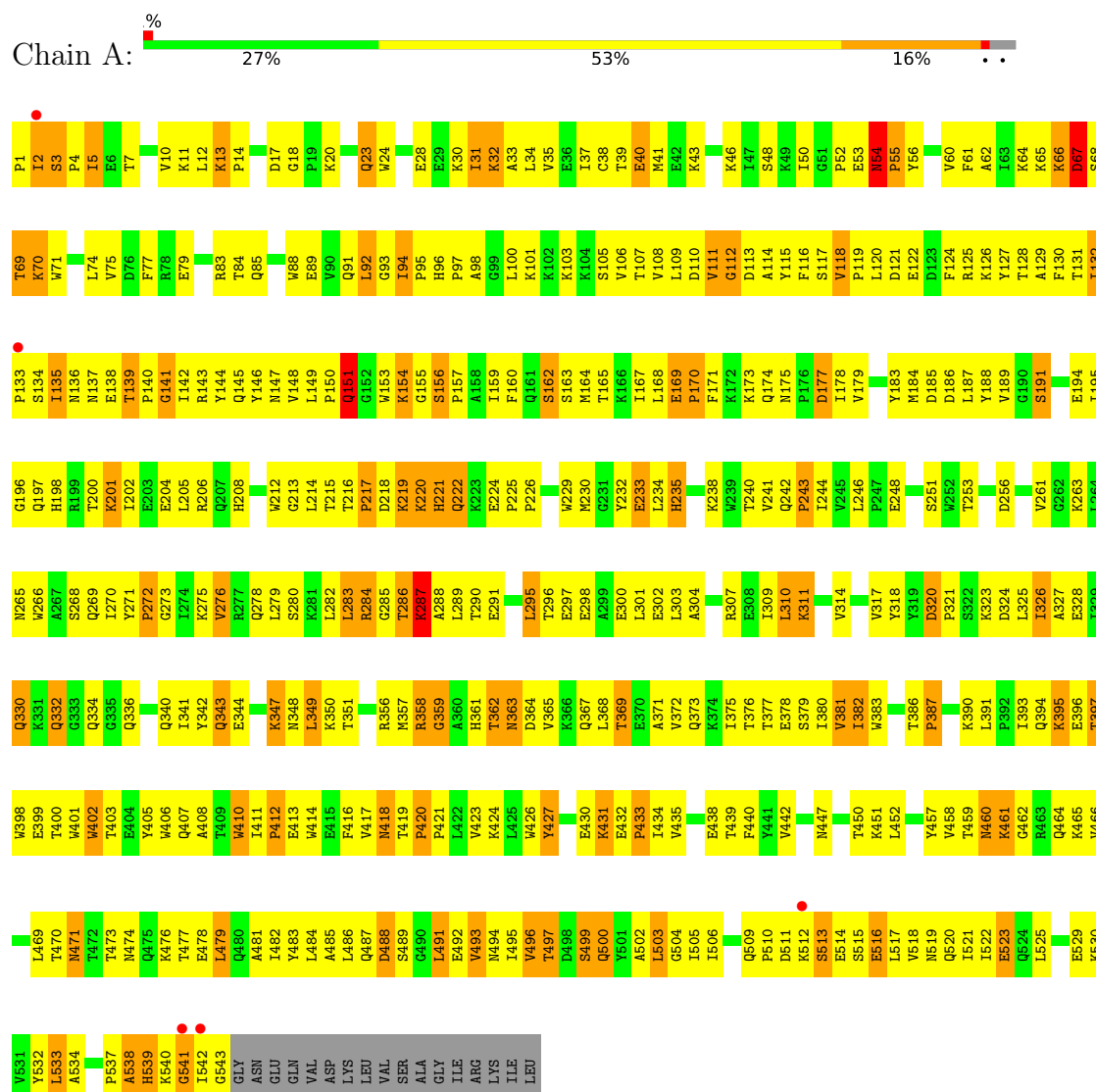
- Molecule 4 is water.

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

3 Residue-property plots

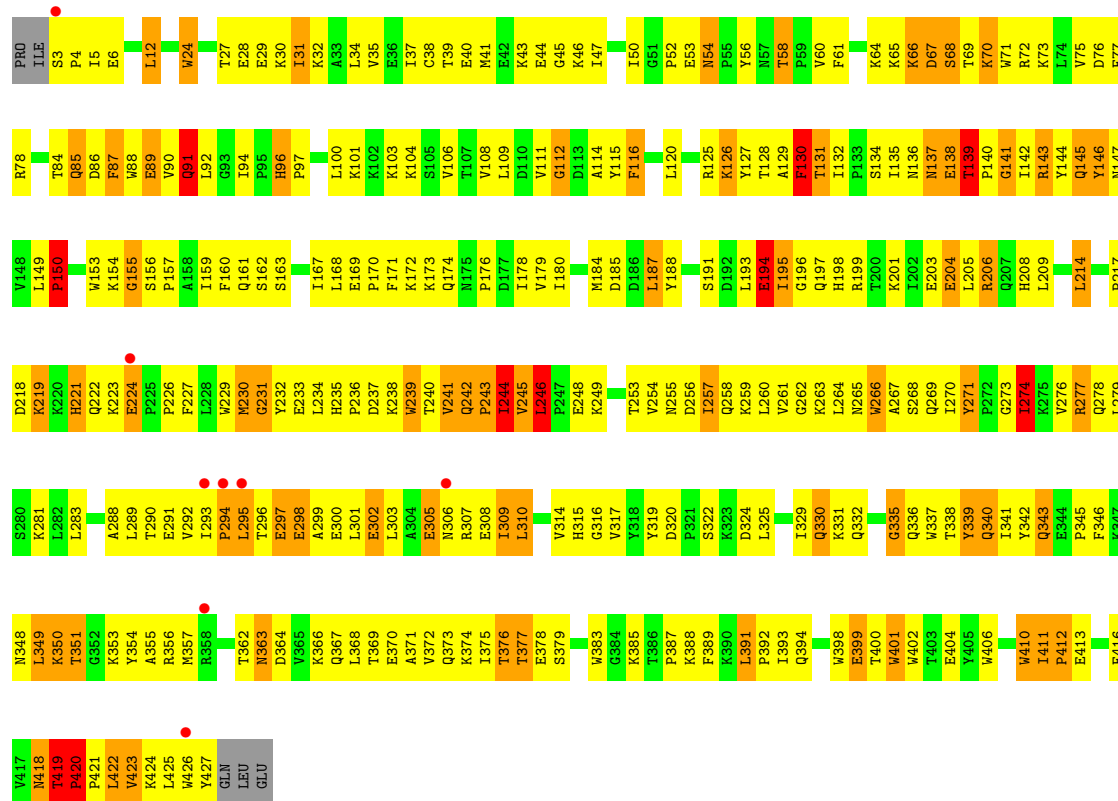
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-2.80) 91.6 (20.00-2.80)	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 0.250 , 0.317	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)	0.27 , 61.1	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

5.1 Standard geometry

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	0.64	0/4547	1.19	50/6178 (0.8%)
2	B	0.80	1/3618 (0.0%)	1.42	62/4918 (1.3%)
All	All	0.72	1/8165 (0.0%)	1.30	112/11096 (1.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	132	ILE	CA-CB	5.01	1.59	1.53

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	GLU	N-CA-C	-14.31	93.64	114.39
2	B	230	MET	N-CA-C	13.52	127.82	110.24
2	B	423	VAL	N-CA-C	-12.82	96.95	112.98
1	A	54	ASN	N-CA-C	-10.39	90.06	108.97
2	B	204	GLU	N-CA-C	-9.93	99.28	111.40
2	B	316	GLY	N-CA-C	-9.85	103.36	115.08
2	B	229	TRP	N-CA-C	9.73	123.76	108.67
1	A	286	THR	N-CA-C	-9.48	90.60	110.80
2	B	219	LYS	N-CA-C	-9.30	98.93	110.65
2	B	194	GLU	N-CA-C	-9.01	96.94	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	ASN	CA-C-N	8.91	129.66	120.04
2	B	54	ASN	C-N-CA	8.91	129.66	120.04
2	B	274	ILE	N-CA-C	8.76	121.21	107.28
2	B	96	HIS	CA-C-N	8.39	130.33	119.84
2	B	96	HIS	C-N-CA	8.39	130.33	119.84
1	A	69	THR	N-CA-C	-8.20	103.42	113.50
2	B	349	LEU	N-CA-C	-8.19	103.08	113.23
2	B	70	LYS	N-CA-C	8.12	122.72	110.14
1	A	359	GLY	N-CA-C	-8.07	94.05	113.18
2	B	245	VAL	N-CA-C	7.81	119.92	107.73
1	A	53	GLU	N-CA-C	7.78	121.98	111.24
1	A	499	SER	N-CA-C	7.56	120.85	108.52
2	B	143	ARG	N-CA-C	7.56	121.22	108.90
2	B	132	ILE	N-CA-C	-7.39	100.30	107.76
2	B	235	HIS	CA-C-N	7.33	128.26	120.12
2	B	235	HIS	C-N-CA	7.33	128.26	120.12
2	B	298	GLU	N-CA-C	-7.29	104.48	113.15
1	A	349	LEU	N-CA-C	-7.03	104.33	113.12
1	A	67	ASP	N-CA-C	-6.99	104.41	114.12
2	B	411	ILE	CA-C-N	-6.93	111.17	119.84
2	B	411	ILE	C-N-CA	-6.93	111.17	119.84
2	B	87	PHE	N-CA-C	-6.90	104.47	113.17
1	A	382	ILE	N-CA-C	6.79	117.40	110.82
2	B	246	LEU	N-CA-C	-6.64	101.13	110.29
2	B	341	ILE	CB-CA-C	-6.54	102.95	110.73
1	A	132	ILE	CA-C-N	6.43	126.41	119.78
1	A	132	ILE	C-N-CA	6.43	126.41	119.78
2	B	267	ALA	N-CA-C	-6.40	104.57	112.38
2	B	244	ILE	N-CA-C	-6.28	96.28	109.34
2	B	343	GLN	N-CA-C	-6.25	107.49	114.62
1	A	512	LYS	N-CA-C	6.19	117.55	108.14
2	B	234	LEU	N-CA-C	-6.16	100.88	110.42
1	A	342	TYR	N-CA-C	6.15	118.12	108.96
2	B	356	ARG	N-CA-C	-6.14	97.71	110.80
1	A	40	GLU	N-CA-C	-6.14	105.75	113.18
2	B	31	ILE	N-CA-C	-6.13	104.54	110.42
1	A	309	ILE	CB-CA-C	-6.10	104.02	112.02
2	B	156	SER	CA-C-N	-6.10	112.57	119.28
2	B	156	SER	C-N-CA	-6.10	112.57	119.28
1	A	533	LEU	N-CA-C	-6.03	99.88	109.76
1	A	13	LYS	CA-C-N	5.95	127.28	119.84
1	A	13	LYS	C-N-CA	5.95	127.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLN	N-CA-C	-5.92	106.09	113.55
2	B	270	ILE	N-CA-C	-5.85	106.78	111.81
2	B	229	TRP	CA-C-N	5.83	129.39	120.82
2	B	229	TRP	C-N-CA	5.83	129.39	120.82
2	B	131	THR	CA-C-N	-5.83	118.39	122.59
2	B	131	THR	C-N-CA	-5.83	118.39	122.59
1	A	106	VAL	N-CA-C	-5.82	100.30	108.27
1	A	2	ILE	N-CA-C	5.78	121.36	109.34
1	A	289	LEU	N-CA-C	5.74	123.03	110.80
1	A	310	LEU	N-CA-C	5.73	117.61	111.36
1	A	286	THR	CA-C-N	5.70	132.43	121.54
1	A	286	THR	C-N-CA	5.70	132.43	121.54
1	A	217	PRO	N-CA-C	-5.63	106.72	113.98
2	B	224	GLU	CA-C-N	5.62	126.17	120.38
2	B	224	GLU	C-N-CA	5.62	126.17	120.38
1	A	493	VAL	N-CA-C	5.61	116.44	108.42
2	B	401	TRP	N-CA-C	5.58	120.37	113.50
2	B	295	LEU	N-CA-C	5.57	115.91	108.23
1	A	500	GLN	N-CA-C	-5.54	105.24	111.28
1	A	391	LEU	N-CA-C	5.50	118.51	110.10
2	B	339	TYR	N-CA-C	5.50	118.15	108.75
1	A	93	GLY	N-CA-C	-5.49	101.85	111.46
2	B	66	LYS	N-CA-C	-5.49	102.02	109.54
2	B	58	THR	N-CA-C	-5.47	102.57	110.40
1	A	24	TRP	CA-C-N	-5.47	114.34	120.14
1	A	24	TRP	C-N-CA	-5.47	114.34	120.14
2	B	420	PRO	N-CA-C	5.46	117.36	110.70
1	A	332	GLN	N-CA-C	-5.44	104.22	111.24
1	A	284	ARG	N-CA-C	-5.43	99.22	110.80
1	A	191	SER	N-CA-C	5.40	115.50	107.88
2	B	293	ILE	CA-C-N	5.40	126.59	119.84
2	B	293	ILE	C-N-CA	5.40	126.59	119.84
2	B	149	LEU	CA-C-N	5.39	126.58	119.84
2	B	149	LEU	C-N-CA	5.39	126.58	119.84
2	B	130	PHE	N-CA-C	-5.39	101.11	109.14
1	A	320	ASP	CA-C-N	5.39	125.46	119.32
1	A	320	ASP	C-N-CA	5.39	125.46	119.32
1	A	118	VAL	CA-C-N	5.38	126.57	119.84
1	A	118	VAL	C-N-CA	5.38	126.57	119.84
2	B	139	THR	N-CA-C	5.35	116.90	108.23
2	B	155	GLY	N-CA-C	-5.34	108.33	115.32
1	A	154	LYS	N-CA-C	5.29	116.85	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	351	THR	N-CA-C	-5.25	102.22	110.36
2	B	94	ILE	CA-C-N	5.24	125.24	119.90
2	B	94	ILE	C-N-CA	5.24	125.24	119.90
1	A	136	ASN	N-CA-C	5.22	121.91	110.80
2	B	416	PHE	N-CA-C	5.19	116.87	108.41
1	A	233	GLU	N-CA-C	-5.16	99.38	108.20
1	A	48	SER	N-CA-C	5.14	117.55	108.75
1	A	179	VAL	N-CA-C	-5.12	100.96	108.85
2	B	391	LEU	N-CA-C	5.12	118.70	109.44
1	A	151	GLN	N-CA-C	5.11	121.69	110.80
2	B	24	TRP	CA-C-N	-5.11	114.65	119.76
2	B	24	TRP	C-N-CA	-5.11	114.65	119.76
1	A	381	VAL	CB-CA-C	-5.10	105.41	112.24
1	A	479	LEU	N-CA-C	-5.06	105.42	112.45
1	A	488	ASP	N-CA-C	5.01	116.74	111.28
2	B	146	TYR	N-CA-C	5.00	118.11	110.20
1	A	391	LEU	CA-C-N	5.00	126.09	119.84
1	A	391	LEU	C-N-CA	5.00	126.09	119.84

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	551	0
2	B	3514	0	3547	420	0
3	A	27	0	14	11	0
4	A	79	0	0	3	0
4	B	63	0	0	1	0
All	All	8112	0	8052	937	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 60.

All (937) 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: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
2:B:297:GLU:HG2	2:B:298:GLU:N	1.56	1.00
1:A:283:LEU:C	1:A:285:GLY:H	1.62	0.99
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
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:199:ARG:HH12	2:B:230:MET:HE3	1.31	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
1:A:285:GLY:C	1:A:287:LYS:H	1.74	0.94
2:B:253:THR:HG22	2:B:292:VAL:HG22	1.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ASN:C	2:B:363:ASN:HD22	1.78	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
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
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
1:A:283:LEU:C	1:A:285:GLY:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:66:LYS:NZ	1:A:66:LYS:HB3	2.00	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
1:A:411:ILE:HG13	1:A:411:ILE:O	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:420:PRO:HA	1:A:421:PRO:C	2.13	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:199:ARG:NH1	2:B:230:MET:HE3	2.03	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
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
1:A:110:ASP:HB3	1:A:218:ASP:CG	2.16	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
2:B:363:ASN:C	2:B:363:ASN:ND2	2.49	0.71
1:A:285:GLY:C	1:A:287:LYS:N	2.37	0.70
1:A:382:ILE:O	2:B:136:ASN:HB2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:332:GLN:HB2	2:B:336:GLN:O	1.91	0.69
2:B:421:PRO:C	2:B:423:VAL:H	2.00	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:419:THR:HG23	1:A:419:THR:O	1.91	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:91:GLN:O	1:A:91:GLN:HG2	1.92	0.67
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
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: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
2:B:243:PRO:C	2:B:245:VAL:H	2.02	0.66
2:B:331:LYS:HZ1	2:B:364:ASP:CG	2.02	0.66
1:A:20:LYS:HG2	1:A:55:PRO:O	1.96	0.66
1:A:69:THR:C	1:A:70:LYS:HD3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:231:GLY:C	2:B:233:GLU:H	2.04	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
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:137:ASN:C	2:B:139:THR:H	2.06	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
2:B:297:GLU:C	2:B:299:ALA:H	2.06	0.63
1:A:101:LYS:HD3	1:A:103:LYS:HZ1	1.61	0.63
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.33	0.63
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:231:GLY:C	2:B:233:GLU:N	2.56	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:447:ASN:HB3	1:A:450:THR:HG1	1.62	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
2:B:278:GLN:HG2	2:B:298:GLU:C	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:B:231:GLY:HA3	2:B:233:GLU:OE2	1.99	0.61
2:B:339:TYR:C	2:B:340:GLN:OE1	2.43	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
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
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:274:ILE:CD1	2:B:306:ASN:HB2	2.31	0.60
2:B:243:PRO:C	2:B:245:VAL:N	2.57	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
1:A:460:ASN:C	1:A:462:GLY:H	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:164:MET:HE3	1:A:187:LEU:CD1	2.32	0.59
1:A:311:LYS:HE2	1:A:311:LYS:C	2.27	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:513:SER:C	1:A:515:SER:H	2.11	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:219:LYS:C	1:A:221:HIS:H	2.10	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: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:271:TYR:C	2:B:273:GLY:H	2.11	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
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
2:B:217:PRO:C	2:B:219:LYS:H	2.11	0.58
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:418:ASN:N	2:B:418:ASN:ND2	2.50	0.58
1:A:317:VAL:CG2	1:A:318:TYR:N	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:369:THR:HG1	1:A:398:TRP:HH2	1.48	0.57
2:B:171:PHE:C	2:B:173:LYS:H	2.10	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:17:ASP:CG	1:A:18:GLY:H	2.11	0.57
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.39	0.57
1:A:394:GLN:O	1:A:395:LYS:C	2.47	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:54:ASN:C	1:A:56:TYR:H	2.12	0.57
1:A:217:PRO:HA	1:A:219:LYS:NZ	2.19	0.57
1:A:298:GLU:H	1:A:298:GLU:CD	2.13	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:315:HIS:C	2:B:317:VAL:H	2.10	0.57
2:B:422:LEU:HB3	2:B:425:LEU:HD12	1.84	0.57
2:B:137:ASN:C	2:B:139:THR:N	2.62	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:GLN:C	2:B:244:ILE:H	2.13	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: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
2:B:171:PHE:C	2:B:173:LYS:N	2.64	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
1:A:217:PRO:HA	1:A:219:LYS:HZ2	1.72	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
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
2:B:146:TYR:CD1	2:B:150:PRO:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:LEU:C	2:B:310:LEU:HD23	2.31	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:131:THR:HG1	2:B:143:ARG:NH1	2.04	0.55
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.41	0.55
1:A:17:ASP:CG	1:A:18:GLY:N	2.65	0.55
2:B:128:THR:O	2:B:129:ALA:C	2.49	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:334:GLN:HB2	1:A:336:GLN:HE21	1.71	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
2:B:173:LYS:O	2:B:176:PRO:HD3	2.06	0.54
2:B:199:ARG:HH12	2:B:230:MET:CE	2.13	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
2:B:331:LYS:NZ	2:B:364:ASP:CG	2.65	0.54
1:A:447:ASN:OD1	1:A:450:THR:HG23	2.07	0.54
2:B:131:THR:HG1	2:B:143:ARG:HH11	1.56	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:183:TYR:CE2	1:A:184:MET:HE2	2.43	0.53
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:370:GLU:O	2:B:371:ALA:C	2.49	0.53
1:A:163:SER:O	1:A:167:ILE:HG13	2.09	0.53
1:A:204:GLU:O	1:A:205:LEU:C	2.51	0.53
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:THR:C	2:B:86:ASP:N	2.66	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:173:LYS:C	1:A:175:ASN:H	2.17	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:216:THR:C	1:A:218:ASP:N	2.64	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:206:ARG:NE	1:A:219:LYS:HA	2.23	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: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
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:257:ILE:O	2:B:258:GLN:C	2.52	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
1:A:504:GLY:O	1:A:505:ILE:C	2.53	0.52
2:B:422:LEU:C	2:B:424:LYS:H	2.16	0.52
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.39	0.52
2:B:87:PHE:C	2:B:88:TRP:HD1	2.18	0.52
2:B:168:LEU:HD21	2:B:209:LEU:HD21	1.91	0.52
2:B:331:LYS:HA	2:B:337:TRP:CE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:CD1	1:A:130:PHE:C	2.88	0.52
1:A:2:ILE:HG22	1:A:4:PRO:HG2	1.87	0.52
1:A:297:GLU:CD	1:A:297:GLU:H	2.17	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:376:THR:O	2:B:377:THR:C	2.53	0.52
2:B:27:THR:O	2:B:31:ILE:HD12	2.10	0.51
2:B:173:LYS:O	2:B:174:GLN:C	2.54	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
1:A:12:LEU:O	1:A:13:LYS:C	2.53	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
2:B:281:LYS:C	2:B:283:LEU:H	2.19	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
1:A:125:ARG:O	1:A:128:THR:OG1	2.29	0.51
1:A:481:ALA:O	1:A:482:ILE:C	2.52	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
2:B:84:THR:C	2:B:86:ASP:H	2.17	0.51
1:A:132:ILE:CG2	1:A:142:ILE:O	2.59	0.51
2:B:90:VAL:C	2:B:92:LEU:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:LEU:HD23	2:B:422:LEU:N	2.24	0.51
2:B:266:TRP:C	2:B:268:SER:N	2.65	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
1:A:85:GLN:C	1:A:154:LYS:HZ3	2.18	0.50
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.46	0.50
1:A:164:MET:HE3	1:A:187:LEU:HD13	1.93	0.50
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.41	0.50
1:A:242:GLN:O	1:A:243:PRO:C	2.54	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
2:B:66:LYS:C	2:B:68:SER:H	2.18	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
1:A:298:GLU:CD	1:A:298:GLU:N	2.69	0.50
1:A:460:ASN:ND2	1:A:460:ASN:N	2.56	0.50
1:A:509:GLN:O	1:A:510:PRO:C	2.55	0.50
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.91	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: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:426:TRP:O	1:A:427:TYR:HB3	2.11	0.49
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:280:SER:C	1:A:282:LEU:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:216:THR:C	1:A:218:ASP:H	2.19	0.49
1:A:410:TRP:CD1	2:B:401:TRP:CD2	3.01	0.49
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
2:B:52:PRO:C	2:B:54:ASN:H	2.20	0.49
2:B:222:GLN:C	2:B:224:GLU:H	2.19	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:212:TRP:C	1:A:214:LEU:H	2.20	0.49
1:A:439:THR:OG1	2:B:289:LEU:HG	2.12	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
2:B:297:GLU:C	2:B:299:ALA:N	2.70	0.48
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.96	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
1:A:221:HIS:O	1:A:222:GLN:C	2.56	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
2:B:306:ASN:C	2:B:308:GLU:H	2.20	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
3:A:701:ABZ:H13	2:B:138:GLU:CD	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG22	1:A:481:ALA:CB	2.40	0.48
2:B:194:GLU:O	2:B:195:ILE:C	2.55	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:306:ASN:C	2:B:308:GLU:N	2.72	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
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:1:PRO:C	1:A:2:ILE:CG1	2.88	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:491:LEU:H	1:A:491:LEU:CD1	2.19	0.47
1:A:519:ASN:O	1:A:523:GLU:HG2	2.15	0.47
2:B:370:GLU:O	2:B:372:VAL:N	2.48	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:23:GLN:CD	1:A:60:VAL:H	2.22	0.47
1:A:40:GLU:OE2	1:A:43:LYS:HD3	2.15	0.47
1:A:174:GLN:O	1:A:175:ASN:CG	2.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:VAL:HG11	2:B:348:ASN:O	2.15	0.47
2:B:332:GLN:HB2	2:B:336:GLN:C	2.39	0.47
2:B:354:TYR:CD1	2:B:355:ALA:N	2.82	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
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: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
2:B:46:LYS:NZ	2:B:116:PHE:CD1	2.77	0.47
2:B:230:MET:O	2:B:231:GLY:C	2.58	0.47
2:B:370:GLU:C	2:B:372:VAL:N	2.72	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
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:513:SER:C	1:A:515:SER:N	2.71	0.46
2:B:44:GLU:OE1	2:B:46:LYS:HE3	2.15	0.46
2:B:140:PRO:O	2:B:141:GLY:C	2.56	0.46
2:B:411:ILE:O	2:B:412:PRO:C	2.54	0.46
1:A:137:ASN:O	1:A:137:ASN:CG	2.58	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
1:A:325:LEU:C	1:A:326:ILE:HD12	2.40	0.46
2:B:43:LYS:C	2:B:45:GLY:N	2.71	0.46
2:B:342:TYR:CD1	2:B:342:TYR:C	2.94	0.46
2:B:367:GLN:O	2:B:370:GLU:HB2	2.15	0.46
2:B:411:ILE:C	2:B:412:PRO:O	2.59	0.46
1:A:168:LEU:O	1:A:169:GLU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:HE2	1:A:488:ASP:OD2	2.16	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:43:LYS:C	2:B:45:GLY:H	2.24	0.46
2:B:160:PHE:O	2:B:161:GLN:C	2.59	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: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:259:LYS:O	2:B:260:LEU:C	2.59	0.45
1:A:253:THR:HG22	1:A:256:ASP:CG	2.41	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
2:B:266:TRP:C	2:B:268:SER:H	2.23	0.45
2:B:320:ASP:OD1	2:B:322:SER:OG	2.34	0.45
1:A:357:MET:O	1:A:358:ARG:C	2.60	0.45
2:B:125:ARG:O	2:B:126:LYS:C	2.59	0.45
2:B:203:GLU:HA	2:B:206:ARG:CB	2.43	0.45
2:B:276:VAL:O	2:B:277:ARG:C	2.59	0.45
2:B:421:PRO:C	2:B:423:VAL:N	2.66	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:447:ASN:CG	1:A:450:THR:HG23	2.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:401:TRP:O	2:B:402:TRP:C	2.60	0.45
1:A:142:ILE:H	1:A:142:ILE:HG13	1.57	0.45
2:B:340:GLN:N	2:B:340:GLN:CD	2.75	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:60:VAL:O	2:B:60:VAL:HG23	2.16	0.44
2:B:90:VAL:C	2:B:92:LEU:N	2.73	0.44
1:A:174:GLN:O	1:A:174:GLN:CD	2.60	0.44
1:A:407:GLN:CG	2:B:393:ILE:HA	2.48	0.44
2:B:260:LEU:C	2:B:262:GLY:N	2.75	0.44
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.16	0.44
2:B:426:TRP:CD1	2:B:426:TRP:C	2.95	0.44
1:A:101:LYS:HE3	1:A:321:PRO:HG3	1.99	0.44
1:A:137:ASN:C	1:A:137:ASN:HD22	2.24	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
1:A:219:LYS:C	1:A:221:HIS:N	2.76	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:169:GLU:C	2:B:171:PHE:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:PHE:HE2	1:A:418:ASN:HB2	1.82	0.44
1:A:460:ASN:C	1:A:462:GLY:N	2.74	0.44
1:A:28:GLU:CA	1:A:31:ILE:HG22	2.46	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
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: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:538:ALA:O	1:A:539:HIS:C	2.61	0.43
2:B:172:LYS:HE2	2:B:172:LYS:HB3	1.81	0.43
2:B:198:HIS:O	2:B:199:ARG:C	2.62	0.43
1:A:115:TYR:O	1:A:149:LEU:HB2	2.18	0.43
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:169:GLU:O	1:A:170:PRO:C	2.62	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
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:28:GLU:C	1:A:31:ILE:CG2	2.91	0.42
1:A:34:LEU:O	1:A:38:CYS:N	2.48	0.42
1:A:120:LEU:O	1:A:121:ASP:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:275:LYS:C	1:A:276:VAL:HG23	2.44	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:68:SER:O	2:B:69:THR:C	2.63	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:397:THR:C	1:A:400:THR:HG22	2.45	0.42
1:A:496:VAL:O	1:A:496:VAL:HG12	2.18	0.42
1:A:125:ARG:NE	1:A:147:ASN:HA	2.32	0.42
1:A:341:ILE:HD11	1:A:375:ILE:HG23	2.00	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
2:B:339:TYR:C	2:B:339:TYR:CD2	2.98	0.42
1:A:54:ASN:C	1:A:56:TYR:N	2.70	0.42
1:A:139:THR:C	1:A:141:GLY:H	2.27	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
2:B:315:HIS:C	2:B:317:VAL:N	2.77	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:61:PHE:O	1:A:62:ALA:C	2.62	0.42
1:A:173:LYS:HB3	1:A:173:LYS:HE2	1.83	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:388:LYS:HE2	4:B:1097:HOH:O	2.20	0.42
1:A:197:GLN:O	1:A:198:HIS:C	2.62	0.42
1:A:235:HIS:CD2	1:A:235:HIS:N	2.87	0.42
2:B:38:CYS:O	2:B:39:THR:C	2.62	0.42
2:B:76:ASP:CG	2:B:78:ARG:HH21	2.28	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
2:B:368:LEU:C	2:B:370:GLU:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TRP:CE3	1:A:402:TRP:C	2.97	0.42
1:A:482:ILE:O	1:A:485:ALA:HB3	2.19	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
1:A:459:THR:O	1:A:460:ASN:C	2.62	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: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
1:A:173:LYS:C	1:A:175:ASN:N	2.76	0.41
1:A:311:LYS:CE	1:A:311:LYS:C	2.90	0.41
1:A:450:THR:C	1:A:451:LYS:HG3	2.43	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: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:164:MET:HE3	1:A:187:LEU:CD2	2.50	0.41
1:A:229:TRP:CZ3	3:A:701:ABZ:H4	2.55	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
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.51	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
1:A:473:THR:O	1:A:474:ASN:C	2.62	0.41
2:B:103:LYS:HD2	2:B:191:SER:HA	2.02	0.41
2:B:205:LEU:O	2:B:206:ARG:C	2.64	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:270:ILE:HG23	1:A:271:TYR:CD1	2.55	0.41
2:B:310:LEU:O	2:B:310:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:350:LYS:HE3	1:A:378:GLU:CD	2.46	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:354:TYR:CD1	2:B:354:TYR:C	2.99	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:271:TYR:C	2:B:273:GLY:N	2.74	0.41
2:B:278:GLN:CG	2:B:298:GLU:C	2.91	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:137:ASN:ND2	1:A:137:ASN:C	2.75	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
1:A:164:MET:CE	1:A:187:LEU:HD22	2.51	0.40
1:A:406:TRP:CE3	1:A:406:TRP:C	3.00	0.40
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
1:A:34:LEU:HB2	1:A:132:ILE:CD1	2.52	0.40
1:A:212:TRP:C	1:A:214:LEU:N	2.80	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:260:LEU:O	2:B:261:VAL:C	2.65	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: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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	541/560 (97%)	415 (77%)	89 (16%)	37 (7%)	1	2
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	B	112	GLY
2	B	243	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	486/500 (97%)	440 (90%)	46 (10%)	8	26
2	B	387/392 (99%)	349 (90%)	38 (10%)	7	25
All	All	873/892 (98%)	789 (90%)	84 (10%)	8	26

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	5	ILE
1	A	23	GLN
1	A	31	ILE
1	A	32	LYS
1	A	54	ASN
1	A	66	LYS
1	A	67	ASP
1	A	70	LYS
1	A	71	TRP
1	A	92	LEU
1	A	94	ILE
1	A	111	VAL
1	A	139	THR
1	A	156	SER
1	A	162	SER
1	A	165	THR
1	A	177	ASP
1	A	201	LYS
1	A	235	HIS
1	A	251	SER

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Mol	Chain	Res	Type
1	A	286	THR
1	A	287	LYS
1	A	295	LEU
1	A	311	LYS
1	A	326	ILE
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	397	THR
1	A	402	TRP
1	A	403	THR
1	A	410	TRP
1	A	413	GLU
1	A	418	ASN
1	A	431	LYS
1	A	460	ASN
1	A	491	LEU
1	A	496	VAL
1	A	497	THR
1	A	514	GLU
1	A	523	GLU
1	A	529	GLU
2	B	12	LEU
2	B	30	LYS
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	145	GLN
2	B	150	PRO
2	B	187	LEU
2	B	194	GLU
2	B	206	ARG
2	B	214	LEU
2	B	221	HIS
2	B	239	TRP
2	B	244	ILE

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Mol	Chain	Res	Type
2	B	246	LEU
2	B	257	ILE
2	B	266	TRP
2	B	271	TYR
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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	91	GLN
1	A	96	HIS
1	A	137	ASN
1	A	269	GLN
1	A	278	GLN
1	A	336	GLN
1	A	460	ASN
1	A	475	GLN
1	A	487	GLN
1	A	494	ASN
1	A	509	GLN
1	A	519	ASN
1	A	520	GLN
2	B	85	GLN
2	B	91	GLN
2	B	136	ASN

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Mol	Chain	Res	Type
2	B	161	GLN
2	B	174	GLN
2	B	197	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	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 oligosaccharides 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	-	30,30,30	1.99	11 (36%)	40,42,42	2.71	15 (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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ABZ	C10-N4	4.36	1.42	1.33
3	A	701	ABZ	C16-C11	3.43	1.45	1.39
3	A	701	ABZ	C8-N3	3.29	1.38	1.33
3	A	701	ABZ	C16-C15	3.28	1.44	1.38
3	A	701	ABZ	C26-N10	-2.64	1.33	1.38
3	A	701	ABZ	C10-N2	2.44	1.39	1.35
3	A	701	ABZ	C13-C12	2.44	1.42	1.38
3	A	701	ABZ	C13-C14	2.35	1.44	1.39
3	A	701	ABZ	C3-N10	-2.34	1.34	1.37
3	A	701	ABZ	C2-C25	2.26	1.52	1.44
3	A	701	ABZ	C12-C11	2.17	1.42	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ABZ	C7-C1-C2	7.06	127.98	120.66
3	A	701	ABZ	C10-N3-C8	6.55	118.58	114.20
3	A	701	ABZ	C2-C3-N10	5.03	109.96	107.09
3	A	701	ABZ	C3-C2-C25	-4.38	103.83	107.02
3	A	701	ABZ	C9-N1-C8	4.29	120.24	114.49
3	A	701	ABZ	N3-C10-N2	-4.18	119.08	125.48
3	A	701	ABZ	N2-C9-N1	-3.87	119.92	126.26
3	A	701	ABZ	C10-N2-C9	3.79	120.06	113.77
3	A	701	ABZ	C3-C2-C1	3.75	123.57	119.57
3	A	701	ABZ	C11-N5-C9	-3.73	119.33	129.38
3	A	701	ABZ	C7-C1-C6	-3.53	117.22	121.98
3	A	701	ABZ	N3-C8-N1	-2.97	122.08	126.09
3	A	701	ABZ	N4-C10-N2	2.70	121.28	117.22
3	A	701	ABZ	C2-C25-C26	-2.39	104.16	106.64
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:

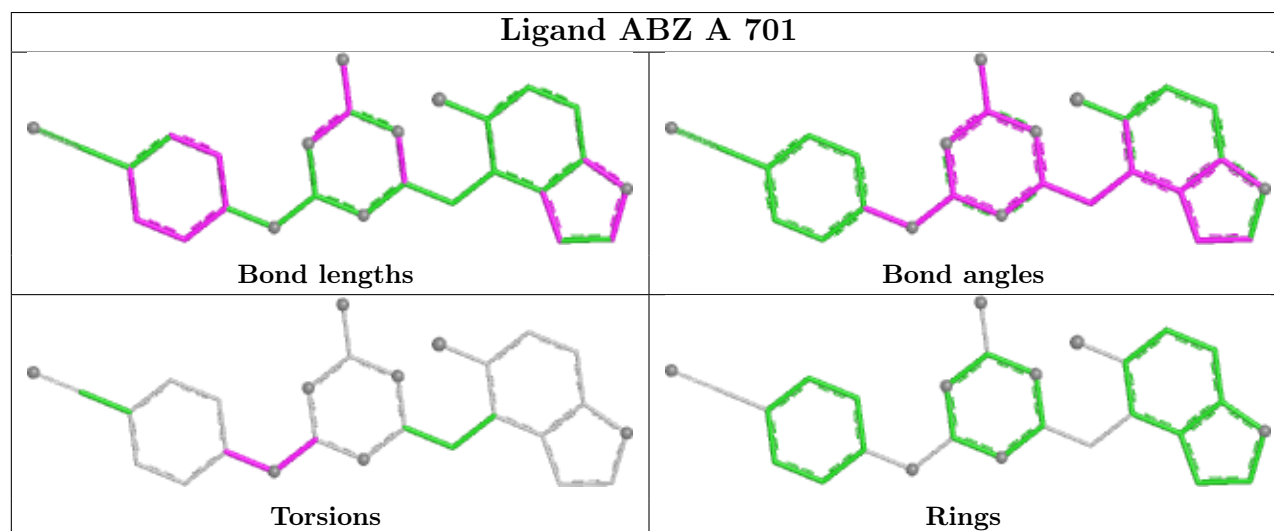
Mol	Chain	Res	Type	Atoms
3	A	701	ABZ	N1-C9-N5-C11
3	A	701	ABZ	N2-C9-N5-C11
3	A	701	ABZ	C16-C11-N5-C9
3	A	701	ABZ	C12-C11-N5-C9

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 ⓘ

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%)	-0.07	5 (0%) 81 74	29, 77, 109, 112	17 (3%)
2	B	425/430 (98%)	-0.16	8 (1%) 66 57	16, 62, 111, 112	14 (3%)
All	All	968/990 (97%)	-0.11	13 (1%) 75 66	16, 73, 111, 112	31 (3%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	GLY	3.3
2	B	293	ILE	3.2
1	A	2	ILE	3.1
1	A	542	ILE	3.0
2	B	306	ASN	2.7
2	B	294	PRO	2.7
2	B	358	ARG	2.5
1	A	133	PRO	2.5
2	B	295	LEU	2.3
2	B	3	SER	2.3
2	B	224	GLU	2.2
2	B	426	TRP	2.2
1	A	512	LYS	2.1

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](#)

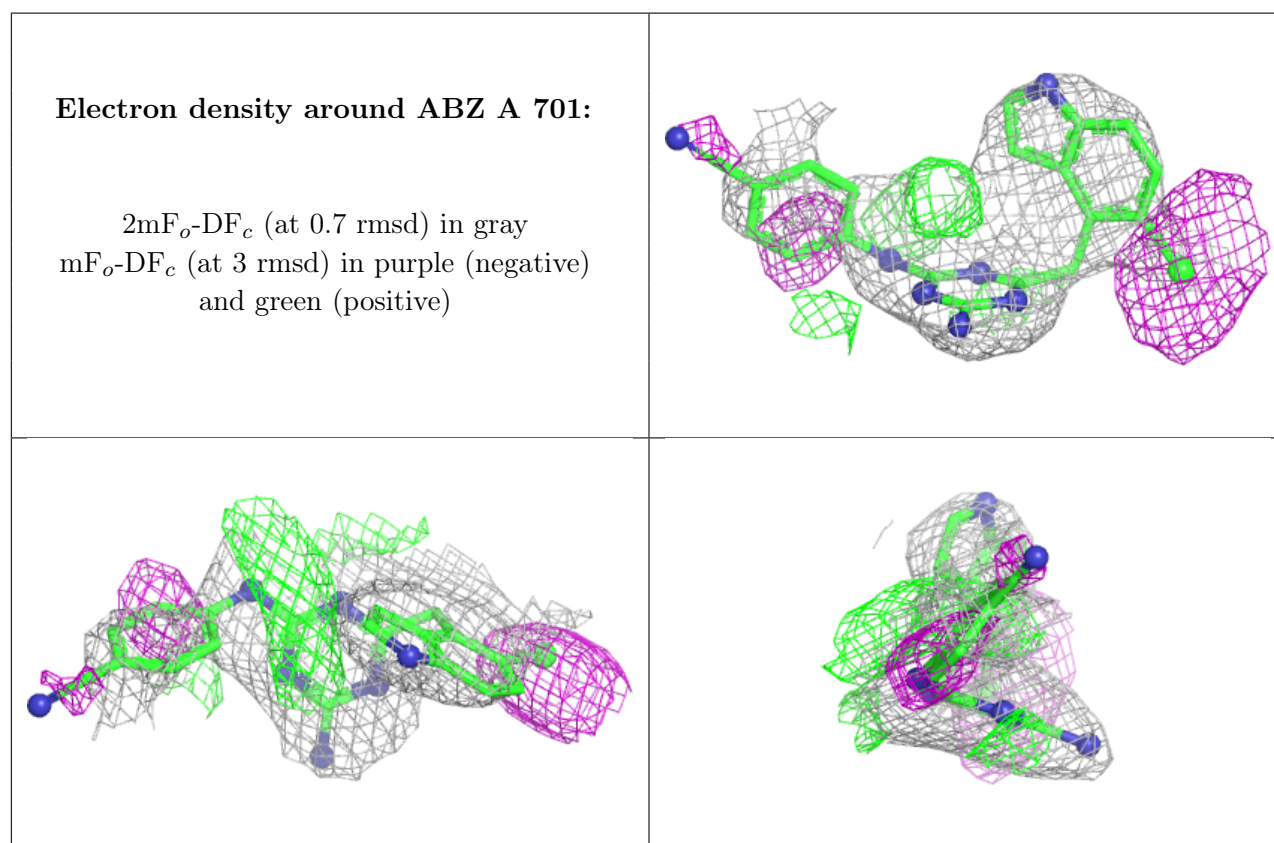
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	ABZ	A	701	27/27	0.69	0.17	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.