



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:21 PM UTC

PDB ID : 1S9E / pdb_00001s9e
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN COMPLEX WITH JANSSEN-R129385
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Deposited on : 2004-02-04
Resolution : 2.60 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

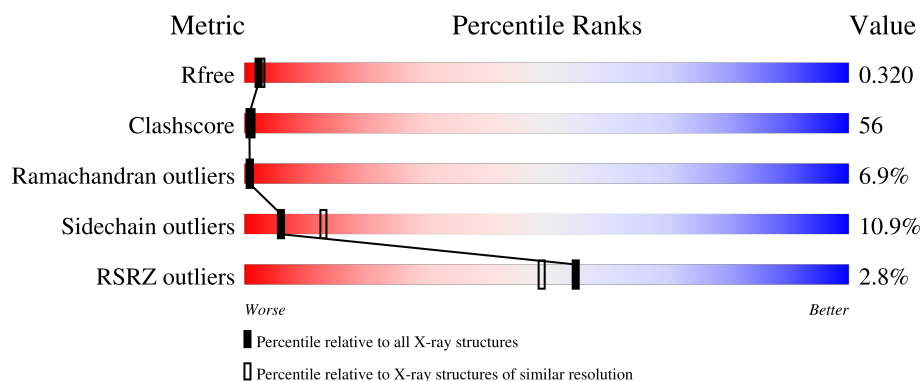
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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% 29% 52% 16% ..
2	B	430	4% 26% 53% 18% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8231 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called POL polyprotein [Contains:Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	122	0	0
			4498	2913	748	830	7			

There is a discrepancy between the modelled and reference sequences:

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

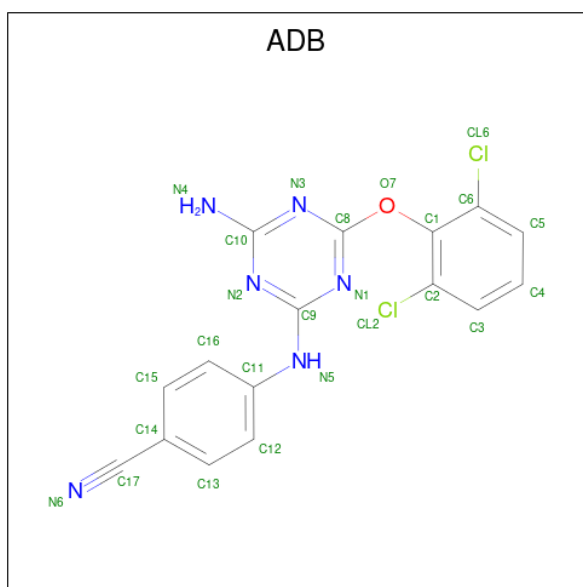
- Molecule 2 is a protein called POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	56	0	0
			3529	2300	584	638	7			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is 4-[4-AMINO-6-(2,6-DICHLORO-PHENOXY)-[1,3,5]TRIAZIN-2-YLAMINO]-BENZONITRILE (CCD ID: ADB) (formula: C₁₆H₁₀Cl₂N₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			25	16	2	6	1		

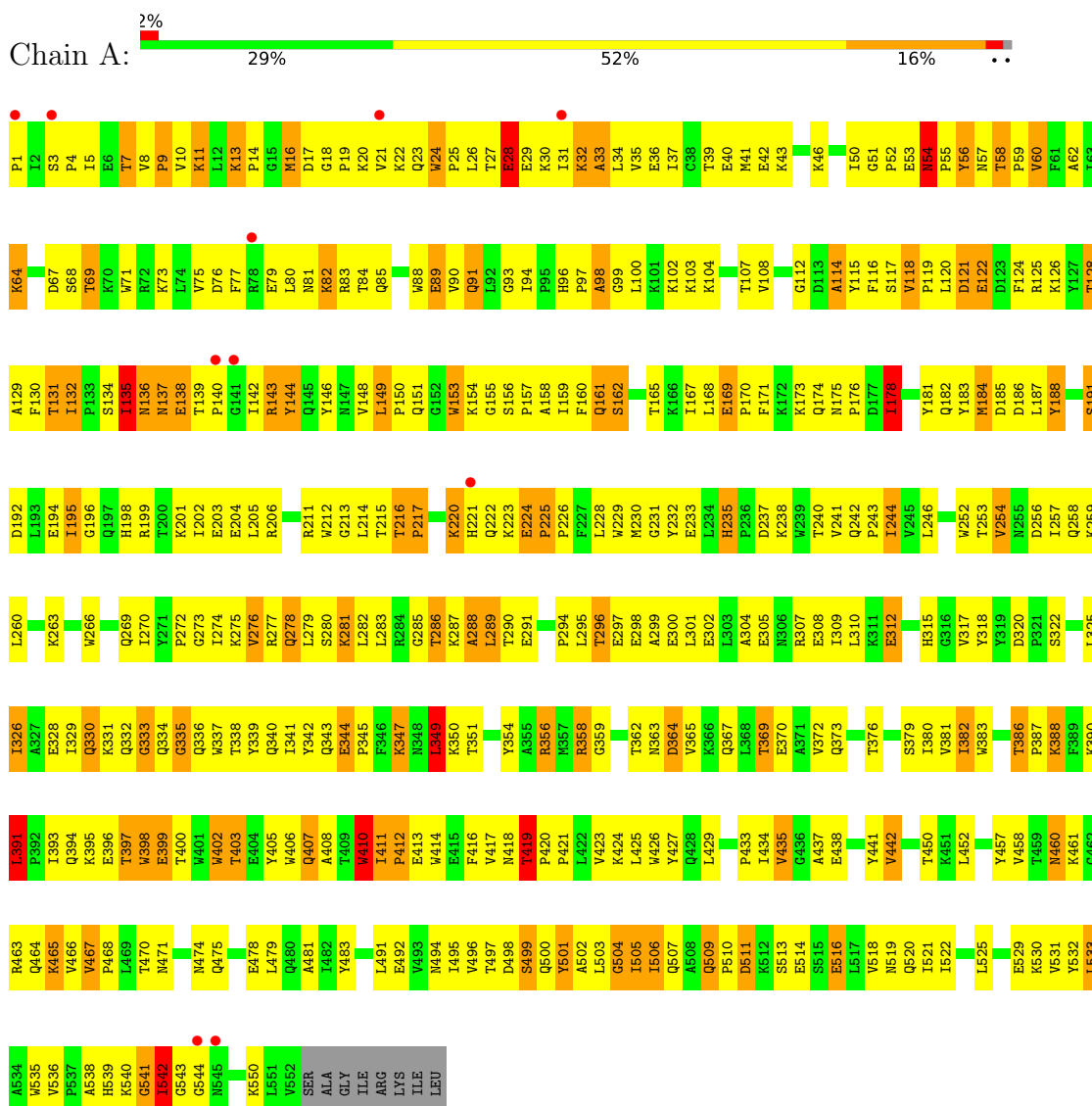
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	94	Total	O	0	0
			94	94		

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]



W398	E399	T400	W401	W402	T403	E404	Y405	W406	W407	A408	T409	W410	W411	E412	E413	W414	E415	F416	W417	M418	T419	P420	P421	L422	L425	W426	Y427	GLN	LEU	GLU																												
K331	Q332	G335	Q336	W337	T338	Y339	Q340	I341	Y342	Q343	E344	P345	F346	K347	N348	Y354	A355	R356	M357	R358	G359	A360	H361	T362	N363	D364	V365	K366	Q367	L368	T369	A370	A371	V372	Q373	K374	L375	T376	T377	E378	S379	I380	V381	I382	K385	K388	F389	K390	L391	P392	I393	Q394	K395	E396	T397			
S268	Q269	I274	K275	V276	R277	Q278	L279	S280	K281	L282	L283	R284	G285	K287	A288	L289	T290	E291	V292	L293	P294	L295	T296	E297	E298	A299	E300	L301	E302	L303	A304	E305	N306	R307	E308	L309	L310	K311	E312	P313	V314	H315	G316	V317	Y318	Y319	D320	P321	S322	K323	D324	L325	L326	G262	A327	E328	I329	Q330
I202	E203	E204	L205	R206	Q207	H208	L209	L214	T215	T216	P217	D218	K219	K220	H221	Q222	K223	E224	P225	P226	F227	L228	W229	H230	G231	Y232	E233	L234	H235	P236	D237	K238	Q242	P243	I244	V245	L246	P247	E248	K249	W252	T253	V254	N255	D256	I257	Q258	K259	L260	V261	G262	N265	W266	A267				
P1	I2	S3	P4	I5	E6	T7	V10	K11	L12	K13	P14	G15	M16	D17	G18	V21	D86	K22	Q23	T27	E28	L92	E29	K30	I31	K32	A33	P34	V35	E36	I37	C38	T39	E40	M41	E42	K43	G45	K46	K49	I50	G51	P52	E53	N54	P55	Y56	T58	P59	V60	F61	A62	I63	K64	K65			
K66	D67	S68	T69	K70	W71	R72	K73	L74	V75	D76	F77	K78	E79	R83	T84	Q85	D86	F87	W88	E89	V90	Q91	L92	G93	I94	P95	H96	P97	A98	K101	K104	S105	L109	D110	V111	G112	D113	A114	Y115	F116	S117	L120	D121	E122	D123	F124	R125	K126	Y127	T128	A129	F130	T131	K65				
P133	S134	I135	N136	M137	E138	T139	P140	R143	Y144	G145	Y146	L149	P150	W153	K154	G155	S156	P157	F160	Q161	S162	S163	M164	P165	K166	I167	L168	E169	P170	F171	K172	K173	D177	I178	V179	I180	Y183	M184	L187	G190	S191	D192	L193	I195	E196	K197	H198	R199	T200	K201								

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.80Å 69.30Å 104.10Å 90.00° 106.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.60) 95.6 (20.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.253 , 0.316 0.259 , 0.320	Depositor DCC
R_{free} test set	2293 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8231	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: ADB

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	0.84	3/4616 (0.1%)	1.36	65/6271 (1.0%)
2	B	0.99	7/3634 (0.2%)	1.43	67/4940 (1.4%)
All	All	0.91	10/8250 (0.1%)	1.39	132/11211 (1.2%)

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	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	35	VAL	CA-CB	-8.67	1.44	1.54
2	B	411	ILE	CA-C	-7.88	1.44	1.52
2	B	135	ILE	CA-CB	-6.37	1.47	1.54
2	B	37	ILE	CA-CB	-6.12	1.47	1.54
1	A	7	THR	CA-CB	5.62	1.62	1.53
2	B	329	ILE	CA-CB	-5.20	1.47	1.54
1	A	533	LEU	CA-C	-5.19	1.46	1.52
1	A	221	HIS	CA-C	5.07	1.56	1.52
2	B	420	PRO	CA-C	5.00	1.56	1.52
2	B	411	ILE	CA-CB	5.00	1.58	1.54

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	GLU	N-CA-C	-14.06	95.98	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	TYR	N-CA-C	-11.59	94.36	110.35
1	A	410	TRP	CA-C-N	-11.51	114.31	122.59
1	A	410	TRP	C-N-CA	-11.51	114.31	122.59
2	B	235	HIS	CA-C-N	11.02	130.62	119.82
2	B	235	HIS	C-N-CA	11.02	130.62	119.82
1	A	333	GLY	N-CA-C	10.62	127.12	114.48
1	A	54	ASN	CA-C-N	-10.31	109.38	119.90
1	A	54	ASN	C-N-CA	-10.31	109.38	119.90
1	A	382	ILE	N-CA-C	10.30	120.81	110.82
2	B	7	THR	N-CA-C	10.25	132.63	110.80
2	B	410	TRP	CA-C-N	-9.83	112.44	123.25
2	B	410	TRP	C-N-CA	-9.83	112.44	123.25
1	A	381	VAL	CB-CA-C	-9.78	99.46	111.97
1	A	118	VAL	CA-C-N	9.64	129.71	119.78
1	A	118	VAL	C-N-CA	9.64	129.71	119.78
1	A	344	GLU	CA-C-N	9.64	131.88	119.84
1	A	344	GLU	C-N-CA	9.64	131.88	119.84
2	B	411	ILE	CA-C-N	-9.14	108.41	119.84
2	B	411	ILE	C-N-CA	-9.14	108.41	119.84
1	A	222	GLN	N-CA-C	9.07	121.44	110.19
2	B	133	PRO	N-CA-C	9.00	123.82	111.22
1	A	13	LYS	CA-C-N	8.96	131.03	119.84
1	A	13	LYS	C-N-CA	8.96	131.03	119.84
1	A	335	GLY	N-CA-C	-8.79	102.81	115.64
1	A	411	ILE	CA-C-N	8.52	130.49	119.84
1	A	411	ILE	C-N-CA	8.52	130.49	119.84
1	A	178	ILE	N-CA-C	8.00	120.06	107.98
1	A	135	ILE	N-CA-C	7.97	125.92	109.34
2	B	225	PRO	N-CA-C	7.58	119.94	110.70
1	A	289	LEU	N-CA-C	-7.33	104.85	114.31
1	A	143	ARG	N-CA-C	7.29	121.29	109.40
2	B	286	THR	N-CA-C	-7.26	101.98	111.71
2	B	94	ILE	CA-C-N	7.25	127.29	119.90
2	B	94	ILE	C-N-CA	7.25	127.29	119.90
2	B	401	TRP	N-CA-C	7.08	122.02	112.88
1	A	312	GLU	CA-C-N	-7.00	113.10	120.03
1	A	312	GLU	C-N-CA	-7.00	113.10	120.03
2	B	194	GLU	N-CA-C	-6.97	100.13	110.23
2	B	419	THR	CA-C-N	-6.95	113.22	120.38
2	B	419	THR	C-N-CA	-6.95	113.22	120.38
1	A	499	SER	N-CA-C	6.87	120.14	107.99
2	B	239	TRP	N-CA-C	-6.86	98.04	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	117	SER	N-CA-C	-6.85	103.82	112.93
2	B	224	GLU	CA-C-N	6.66	127.24	120.38
2	B	224	GLU	C-N-CA	6.66	127.24	120.38
2	B	204	GLU	N-CA-C	-6.66	104.10	111.36
1	A	349	LEU	N-CA-C	-6.64	104.82	113.12
1	A	191	SER	N-CA-C	6.63	116.81	108.45
2	B	397	THR	N-CA-C	-6.60	104.01	111.07
2	B	249	LYS	N-CA-C	6.59	120.26	109.06
1	A	281	LYS	N-CA-C	-6.59	104.14	111.71
1	A	467	VAL	CA-C-N	6.55	126.78	119.90
1	A	467	VAL	C-N-CA	6.55	126.78	119.90
2	B	171	PHE	N-CA-C	-6.54	104.48	113.18
2	B	122	GLU	N-CA-C	6.53	118.40	111.28
1	A	221	HIS	N-CA-C	6.52	121.06	111.34
1	A	144	TYR	N-CA-C	6.48	120.09	109.85
2	B	143	ARG	N-CA-C	6.48	119.71	108.76
1	A	286	THR	N-CA-C	6.32	122.09	113.37
2	B	382	ILE	CB-CA-C	-6.30	104.00	111.94
1	A	26	LEU	N-CA-C	6.22	118.56	107.80
2	B	410	TRP	N-CA-C	6.21	119.32	109.81
2	B	391	LEU	N-CA-C	6.16	120.37	109.58
2	B	88	TRP	N-CA-C	-6.14	103.26	112.54
2	B	237	ASP	N-CA-C	-6.14	105.62	113.23
1	A	511	ASP	N-CA-C	-6.12	104.17	111.69
1	A	442	VAL	N-CA-C	6.09	117.95	109.55
2	B	31	ILE	N-CA-CB	6.05	117.23	110.51
1	A	114	ALA	N-CA-C	6.05	118.40	111.02
1	A	136	ASN	N-CA-C	6.00	123.57	110.80
2	B	31	ILE	CB-CA-C	-5.99	104.22	111.88
1	A	69	THR	N-CA-C	-5.97	98.08	110.80
2	B	208	HIS	N-CA-C	-5.97	104.69	111.07
2	B	236	PRO	N-CA-C	5.86	121.54	113.98
2	B	238	LYS	N-CA-C	-5.85	105.73	112.92
2	B	327	ALA	N-CA-C	5.83	117.94	108.26
2	B	96	HIS	N-CA-C	5.79	117.84	109.04
1	A	550	LYS	N-CA-C	-5.70	105.16	111.71
2	B	165	THR	N-CA-C	-5.65	104.33	111.11
1	A	509	GLN	CA-C-N	5.64	126.89	119.84
1	A	509	GLN	C-N-CA	5.64	126.89	119.84
1	A	138	GLU	N-CA-C	-5.64	98.79	110.80
2	B	56	TYR	N-CA-C	5.59	118.10	110.55
2	B	362	THR	N-CA-C	5.58	117.88	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	LYS	N-CA-C	-5.55	101.50	110.32
2	B	131	THR	N-CA-C	5.55	117.45	108.41
2	B	419	THR	N-CA-C	5.54	122.06	109.81
1	A	419	THR	CA-C-N	5.52	126.07	120.38
1	A	419	THR	C-N-CA	5.52	126.07	120.38
2	B	70	LYS	N-CA-C	5.50	117.16	108.96
2	B	416	PHE	N-CA-C	5.50	117.93	109.07
1	A	67	ASP	CA-C-N	5.50	129.05	120.75
1	A	67	ASP	C-N-CA	5.50	129.05	120.75
1	A	235	HIS	CA-C-N	5.49	126.70	119.84
1	A	235	HIS	C-N-CA	5.49	126.70	119.84
1	A	359	GLY	N-CA-C	5.49	121.77	112.22
2	B	316	GLY	N-CA-C	-5.49	108.06	115.36
2	B	172	LYS	N-CA-C	-5.49	105.85	112.54
2	B	421	PRO	N-CA-C	5.48	123.75	112.47
1	A	42	GLU	N-CA-C	-5.47	105.39	111.36
2	B	131	THR	CB-CA-C	-5.46	101.09	110.16
1	A	33	ALA	N-CA-C	-5.44	104.77	111.40
2	B	96	HIS	CA-C-N	5.43	126.28	119.98
2	B	96	HIS	C-N-CA	5.43	126.28	119.98
2	B	155	GLY	N-CA-C	-5.42	100.33	113.18
2	B	168	LEU	N-CA-C	5.40	119.58	112.89
1	A	405	TYR	N-CA-C	5.39	118.13	110.10
2	B	104	LYS	N-CA-C	-5.38	106.56	113.01
1	A	225	PRO	N-CA-C	5.35	117.23	110.70
1	A	11	LYS	N-CA-C	5.33	117.36	108.99
1	A	391	LEU	N-CA-C	5.32	117.81	108.82
2	B	348	ASN	N-CA-C	5.27	117.34	109.59
2	B	130	PHE	N-CA-C	-5.27	101.17	109.50
2	B	411	ILE	N-CA-C	5.25	113.35	108.15
2	B	30	LYS	CA-C-N	-5.21	113.87	120.60
2	B	30	LYS	C-N-CA	-5.21	113.87	120.60
2	B	59	PRO	N-CA-C	5.21	119.22	111.41
2	B	149	LEU	CA-C-N	-5.21	113.33	119.84
2	B	149	LEU	C-N-CA	-5.21	113.33	119.84
1	A	278	GLN	N-CA-C	5.20	117.95	111.24
1	A	64	LYS	N-CA-C	-5.17	99.79	110.80
1	A	43	LYS	N-CA-C	-5.08	105.63	111.07
1	A	381	VAL	N-CA-CB	5.08	116.50	110.55
1	A	233	GLU	N-CA-C	-5.08	99.01	107.80
1	A	149	LEU	CA-C-N	5.08	126.18	119.84
1	A	149	LEU	C-N-CA	5.08	126.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ALA	N-CA-C	5.06	116.86	110.33
2	B	66	LYS	N-CA-C	-5.05	100.05	110.80
2	B	420	PRO	CA-C-N	5.04	126.14	119.84
2	B	420	PRO	C-N-CA	5.04	126.14	119.84
2	B	354	TYR	N-CA-C	-5.03	102.34	110.14

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	PHE	Sidechain
2	B	144	TYR	Sidechain
2	B	318	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4498	0	4560	506	0
2	B	3529	0	3568	404	0
3	A	25	0	10	4	0
4	A	85	0	0	4	0
4	B	94	0	0	18	0
All	All	8231	0	8138	887	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 56.

All (887) 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:244:ILE:HD11	1:A:310:LEU:HD13	1.26	1.14
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.31	1.09
2:B:278:GLN:HA	2:B:281:LYS:HE3	1.30	1.09
2:B:363:ASN:C	2:B:363:ASN:HD22	1.63	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.38	1.04
1:A:497:THR:HG22	1:A:499:SER:H	1.21	1.04
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.16	1.04
2:B:277:ARG:H	2:B:277:ARG:HD3	1.18	1.03
2:B:363:ASN:ND2	2:B:366:LYS:H	1.59	1.00
1:A:288:ALA:CB	1:A:291:GLU:HB2	1.91	0.98
2:B:5:ILE:HG22	2:B:6:GLU:H	1.29	0.98
2:B:65:LYS:HA	2:B:72:ARG:HG3	1.46	0.97
2:B:221:HIS:CE1	2:B:230:MET:HG2	2.01	0.95
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.45	0.95
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.05	0.94
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.50	0.94
1:A:22:LYS:HG2	1:A:24:TRP:CZ2	2.03	0.94
2:B:363:ASN:HD21	2:B:366:LYS:H	1.02	0.93
2:B:282:LEU:HG	2:B:293:ILE:HD11	1.47	0.92
1:A:503:LEU:HG	1:A:507:GLN:NE2	1.85	0.92
1:A:460:ASN:N	1:A:460:ASN:HD22	1.66	0.91
2:B:274:ILE:HG23	2:B:306:ASN:OD1	1.70	0.91
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.53	0.90
1:A:542:ILE:HD13	1:A:544:GLY:H	1.36	0.90
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.35	0.90
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.37	0.90
1:A:96:HIS:HD2	1:A:98:ALA:H	1.17	0.89
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.53	0.89
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.02	0.89
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.56	0.88
2:B:362:THR:CG2	2:B:367:GLN:HE21	1.87	0.88
1:A:506:ILE:HG21	1:A:533:LEU:HD12	1.54	0.87
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.58	0.86
2:B:303:LEU:O	2:B:307:ARG:HB2	1.75	0.86
2:B:310:LEU:O	2:B:310:LEU:HD23	1.76	0.86
1:A:90:VAL:HG12	1:A:91:GLN:HG3	1.57	0.86
1:A:226:PRO:HG3	1:A:235:HIS:CE1	2.11	0.86
1:A:465:LYS:HG3	1:A:466:VAL:N	1.88	0.86
2:B:278:GLN:NE2	2:B:298:GLU:HB2	1.91	0.86
2:B:363:ASN:HD21	2:B:366:LYS:N	1.73	0.85
2:B:31:ILE:O	2:B:35:VAL:HG23	1.75	0.85
1:A:406:TRP:CZ3	2:B:420:PRO:HD2	2.10	0.85
1:A:388:LYS:NZ	1:A:413:GLU:HG3	1.92	0.85
2:B:244:ILE:O	2:B:310:LEU:HD21	1.76	0.85
1:A:104:LYS:HE2	1:A:104:LYS:N	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASN:HD22	1:A:460:ASN:H	1.25	0.84
1:A:497:THR:HG22	1:A:498:ASP:N	1.89	0.84
1:A:148:VAL:O	1:A:150:PRO:HD3	1.77	0.84
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.77	0.84
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.59	0.84
1:A:224:GLU:HB3	1:A:225:PRO:CD	2.07	0.84
1:A:254:VAL:O	1:A:257:ILE:HG22	1.78	0.84
1:A:542:ILE:HG12	1:A:543:GLY:H	1.43	0.83
1:A:206:ARG:HH22	1:A:217:PRO:C	1.86	0.83
2:B:422:LEU:HD12	2:B:425:LEU:HD12	1.61	0.83
1:A:104:LYS:HG2	1:A:192:ASP:HA	1.61	0.82
1:A:298:GLU:H	1:A:298:GLU:CD	1.87	0.82
1:A:53:GLU:C	1:A:55:PRO:HD3	2.03	0.82
1:A:435:VAL:CG1	2:B:290:THR:HG21	2.07	0.82
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.59	0.81
1:A:96:HIS:CD2	1:A:98:ALA:H	1.99	0.81
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.15	0.81
1:A:46:LYS:HD3	1:A:116:PHE:HB3	1.62	0.81
2:B:221:HIS:NE2	2:B:230:MET:HE3	1.96	0.81
1:A:64:LYS:HE3	1:A:68:SER:HB3	1.62	0.81
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.15	0.81
2:B:249:LYS:HD2	2:B:252:TRP:CZ3	2.16	0.81
1:A:155:GLY:O	1:A:159:ILE:HG13	1.81	0.80
2:B:206:ARG:HB3	2:B:206:ARG:NH1	1.96	0.80
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.80	0.80
2:B:296:THR:OG1	2:B:299:ALA:HB2	1.83	0.79
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.65	0.79
2:B:85:GLN:HG2	4:B:1089:HOH:O	1.81	0.79
1:A:224:GLU:CB	1:A:225:PRO:HD2	2.11	0.78
1:A:136:ASN:O	1:A:138:GLU:N	2.16	0.78
1:A:388:LYS:HZ3	1:A:413:GLU:HG3	1.47	0.78
1:A:287:LYS:HG2	1:A:288:ALA:H	1.49	0.77
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.67	0.77
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.15	0.77
1:A:138:GLU:HA	1:A:138:GLU:OE2	1.85	0.77
1:A:220:LYS:HB2	4:A:1009:HOH:O	1.85	0.77
1:A:540:LYS:HD2	2:B:265:ASN:ND2	2.00	0.77
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.50	0.76
1:A:115:TYR:HD2	1:A:149:LEU:O	1.69	0.76
1:A:315:HIS:CE1	1:A:347:LYS:HD3	2.20	0.76
1:A:19:PRO:HG3	1:A:80:LEU:HA	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.21	0.76
1:A:139:THR:HB	1:A:140:PRO:HD2	1.66	0.76
1:A:506:ILE:HG21	1:A:533:LEU:CD1	2.15	0.76
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.21	0.75
1:A:13:LYS:HD2	1:A:16:MET:HE3	1.68	0.75
1:A:181:TYR:HE2	1:A:183:TYR:HB2	1.50	0.75
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.68	0.75
1:A:506:ILE:HG22	1:A:507:GLN:N	2.00	0.75
2:B:222:GLN:HG2	2:B:223:LYS:HG2	1.68	0.75
1:A:97:PRO:HG2	1:A:232:TYR:CE2	2.22	0.75
1:A:287:LYS:H	1:A:287:LYS:HD3	1.51	0.75
1:A:1:PRO:O	1:A:117:SER:HA	1.87	0.75
1:A:10:VAL:HG12	1:A:11:LYS:N	2.02	0.74
2:B:366:LYS:HG3	2:B:405:TYR:CG	2.22	0.74
2:B:298:GLU:HB3	2:B:301:LEU:HD13	1.69	0.74
1:A:103:LYS:C	1:A:104:LYS:HE2	2.12	0.74
1:A:183:TYR:CE2	1:A:230:MET:SD	2.81	0.74
1:A:503:LEU:HG	1:A:507:GLN:HE22	1.51	0.74
1:A:509:GLN:N	1:A:510:PRO:HD3	2.02	0.74
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.23	0.74
1:A:96:HIS:HD2	1:A:98:ALA:N	1.85	0.74
1:A:497:THR:HG22	1:A:499:SER:N	2.01	0.74
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.68	0.74
1:A:417:VAL:HG12	1:A:419:THR:HG23	1.68	0.74
1:A:337:TRP:NE1	1:A:367:GLN:HE21	1.85	0.74
1:A:312:GLU:O	1:A:312:GLU:HG2	1.89	0.73
2:B:356:ARG:HG2	2:B:362:THR:HG21	1.69	0.73
1:A:540:LYS:HD2	2:B:265:ASN:HD21	1.52	0.73
2:B:356:ARG:HG3	2:B:357:MET:H	1.52	0.73
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.18	0.73
2:B:27:THR:CG2	2:B:29:GLU:HB3	2.19	0.73
1:A:28:GLU:HB3	1:A:135:ILE:HD13	1.71	0.73
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.22	0.73
1:A:382:ILE:HG23	2:B:136:ASN:ND2	2.04	0.73
1:A:542:ILE:HG12	1:A:543:GLY:N	2.04	0.73
1:A:438:GLU:HG3	1:A:460:ASN:HD21	1.54	0.72
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.70	0.72
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.71	0.72
2:B:278:GLN:HE22	2:B:298:GLU:HB2	1.53	0.72
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.55	0.72
1:A:435:VAL:HG13	2:B:290:THR:CG2	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:HD2	1:A:143:ARG:HH12	1.55	0.71
2:B:362:THR:HG22	2:B:367:GLN:NE2	2.00	0.71
1:A:253:THR:OG1	1:A:290:THR:HA	1.90	0.71
1:A:64:LYS:HE3	1:A:68:SER:CB	2.21	0.71
1:A:424:LYS:HD3	1:A:425:LEU:N	2.05	0.71
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.31	0.71
2:B:278:GLN:OE1	2:B:297:GLU:HB2	1.90	0.71
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.20	0.71
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.26	0.71
2:B:345:PRO:HB2	2:B:346:PHE:HD1	1.54	0.71
1:A:301:LEU:O	1:A:305:GLU:HG3	1.90	0.70
2:B:221:HIS:HE1	2:B:230:MET:HG2	1.55	0.70
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.26	0.70
1:A:542:ILE:HD13	1:A:544:GLY:N	2.06	0.70
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.74	0.70
1:A:30:LYS:O	1:A:33:ALA:N	2.25	0.70
1:A:507:GLN:O	1:A:509:GLN:HG3	1.91	0.70
2:B:278:GLN:HA	2:B:281:LYS:CE	2.18	0.70
1:A:373:GLN:OE1	2:B:397:THR:HA	1.91	0.70
1:A:495:ILE:HB	1:A:533:LEU:HD23	1.74	0.70
2:B:298:GLU:HB3	2:B:301:LEU:CD1	2.22	0.69
2:B:418:ASN:O	2:B:419:THR:HG23	1.92	0.69
1:A:298:GLU:CD	1:A:298:GLU:N	2.50	0.69
1:A:33:ALA:O	1:A:37:ILE:HG12	1.92	0.69
1:A:225:PRO:HA	1:A:226:PRO:C	2.17	0.69
2:B:76:ASP:CG	2:B:78:ARG:HH21	2.00	0.69
1:A:277:ARG:HD2	1:A:334:GLN:CB	2.23	0.69
1:A:497:THR:CG2	1:A:499:SER:H	2.03	0.69
1:A:277:ARG:HD2	1:A:334:GLN:HB3	1.75	0.68
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.74	0.68
1:A:27:THR:O	1:A:29:GLU:N	2.25	0.68
1:A:518:VAL:O	1:A:522:ILE:HG13	1.94	0.68
2:B:339:TYR:C	2:B:340:GLN:OE1	2.36	0.68
1:A:376:THR:HG23	1:A:386:THR:HG22	1.75	0.68
2:B:371:ALA:O	2:B:375:ILE:HG13	1.93	0.68
1:A:331:LYS:NZ	1:A:333:GLY:HA2	2.09	0.68
1:A:373:GLN:HG2	2:B:394:GLN:NE2	2.09	0.68
2:B:277:ARG:HD3	2:B:277:ARG:N	2.00	0.68
1:A:398:TRP:NE1	1:A:402:TRP:HD1	1.92	0.68
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.74	0.68
1:A:474:ASN:O	1:A:478:GLU:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:O	1:A:286:THR:HG22	1.93	0.67
1:A:244:ILE:HD11	1:A:310:LEU:CD1	2.15	0.67
1:A:326:ILE:HD12	1:A:326:ILE:N	2.09	0.67
1:A:420:PRO:HA	1:A:421:PRO:C	2.18	0.67
2:B:357:MET:HB2	2:B:361:HIS:HE2	1.59	0.67
2:B:76:ASP:OD1	2:B:78:ARG:NE	2.20	0.67
1:A:354:TYR:OH	1:A:356:ARG:HD3	1.94	0.67
2:B:101:LYS:O	2:B:236:PRO:HB2	1.95	0.67
2:B:388:LYS:HE3	2:B:415:GLU:OE1	1.95	0.67
1:A:542:ILE:CD1	1:A:544:GLY:H	2.07	0.67
2:B:363:ASN:C	2:B:363:ASN:ND2	2.39	0.67
1:A:29:GLU:OE1	1:A:29:GLU:HA	1.94	0.66
2:B:257:ILE:O	2:B:261:VAL:HG23	1.95	0.66
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.10	0.66
1:A:301:LEU:O	1:A:301:LEU:HD12	1.95	0.66
2:B:357:MET:HB2	2:B:361:HIS:NE2	2.10	0.66
2:B:5:ILE:HG22	2:B:6:GLU:N	2.08	0.66
2:B:411:ILE:O	2:B:412:PRO:C	2.37	0.66
2:B:278:GLN:HE22	2:B:298:GLU:CB	2.07	0.66
1:A:417:VAL:HG12	1:A:417:VAL:O	1.96	0.66
2:B:86:ASP:O	2:B:89:GLU:HB3	1.95	0.66
1:A:460:ASN:N	1:A:460:ASN:ND2	2.40	0.66
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.32	0.65
1:A:27:THR:O	1:A:30:LYS:N	2.28	0.65
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.76	0.65
2:B:23:GLN:HB2	4:B:1090:HOH:O	1.95	0.65
2:B:278:GLN:HE22	2:B:298:GLU:CG	2.09	0.65
2:B:422:LEU:O	2:B:425:LEU:HB2	1.96	0.65
1:A:10:VAL:HG12	1:A:11:LYS:H	1.59	0.65
1:A:434:ILE:H	1:A:494:ASN:HD21	1.43	0.65
1:A:81:ASN:C	1:A:83:ARG:H	2.03	0.65
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.27	0.65
1:A:315:HIS:NE2	1:A:347:LYS:HD3	2.11	0.65
2:B:53:GLU:OE1	2:B:53:GLU:N	2.29	0.65
1:A:290:THR:O	1:A:290:THR:HG22	1.96	0.64
1:A:363:ASN:OD1	1:A:365:VAL:N	2.30	0.64
1:A:56:TYR:CD1	1:A:56:TYR:N	2.64	0.64
2:B:411:ILE:HA	4:B:1088:HOH:O	1.97	0.64
1:A:279:LEU:CD2	1:A:299:ALA:HB1	2.25	0.64
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.62	0.64
2:B:46:LYS:CE	2:B:116:PHE:HD1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:GLY:O	2:B:355:ALA:HA	1.97	0.64
2:B:85:GLN:HA	4:B:1089:HOH:O	1.98	0.63
1:A:270:ILE:O	1:A:272:PRO:HD3	1.98	0.63
2:B:156:SER:N	2:B:157:PRO:HD2	2.13	0.63
2:B:46:LYS:HD3	2:B:116:PHE:CD1	2.33	0.63
1:A:433:PRO:HG3	2:B:255:ASN:HD22	1.63	0.63
2:B:278:GLN:NE2	2:B:298:GLU:CB	2.61	0.63
1:A:373:GLN:HG2	2:B:394:GLN:HE22	1.64	0.63
1:A:497:THR:CG2	1:A:498:ASP:N	2.59	0.63
2:B:359:GLY:O	2:B:361:HIS:N	2.32	0.63
2:B:362:THR:HG23	2:B:366:LYS:HZ2	1.64	0.63
1:A:50:ILE:HG13	1:A:51:GLY:N	2.13	0.63
2:B:195:ILE:HG23	2:B:196:GLY:N	2.13	0.62
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.17	0.62
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.00	0.62
1:A:400:THR:O	1:A:403:THR:HB	1.99	0.62
2:B:217:PRO:O	2:B:219:LYS:N	2.32	0.62
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.23	0.62
2:B:305:GLU:HG3	2:B:306:ASN:N	2.14	0.62
1:A:35:VAL:O	1:A:39:THR:HG23	1.98	0.62
1:A:287:LYS:H	1:A:287:LYS:CD	2.12	0.62
2:B:357:MET:CB	2:B:361:HIS:HE2	2.13	0.62
1:A:27:THR:O	1:A:27:THR:HG22	1.99	0.62
1:A:492:GLU:OE1	1:A:530:LYS:HD2	2.00	0.62
1:A:501:TYR:O	1:A:505:ILE:HD12	1.99	0.62
2:B:282:LEU:CG	2:B:293:ILE:HD11	2.27	0.62
2:B:308:GLU:C	2:B:310:LEU:H	2.06	0.62
2:B:373:GLN:HG2	2:B:406:TRP:CH2	2.35	0.62
1:A:474:ASN:HD22	1:A:474:ASN:H	1.48	0.62
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.35	0.62
2:B:342:TYR:CD1	2:B:342:TYR:C	2.78	0.62
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.28	0.61
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.15	0.61
1:A:442:VAL:HG13	1:A:481:ALA:CB	2.30	0.61
1:A:10:VAL:CG1	1:A:11:LYS:H	2.14	0.61
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.26	0.61
2:B:221:HIS:NE2	2:B:230:MET:HG2	2.16	0.61
2:B:224:GLU:O	2:B:226:PRO:HD3	2.00	0.61
1:A:121:ASP:O	1:A:122:GLU:C	2.43	0.61
1:A:3:SER:HB3	1:A:212:TRP:C	2.26	0.61
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TRP:CD1	1:A:402:TRP:HD1	2.18	0.61
2:B:87:PHE:O	2:B:91:GLN:HB2	2.00	0.60
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.87	0.60
2:B:255:ASN:O	2:B:258:GLN:HB2	2.01	0.60
1:A:90:VAL:HG12	1:A:91:GLN:CG	2.28	0.60
1:A:115:TYR:CD2	1:A:149:LEU:O	2.54	0.60
2:B:369:THR:O	2:B:373:GLN:HG3	2.00	0.60
1:A:102:LYS:HG2	1:A:104:LYS:NZ	2.17	0.60
1:A:258:GLN:HG2	1:A:283:LEU:HD21	1.83	0.60
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.84	0.60
2:B:253:THR:HA	2:B:292:VAL:HA	1.84	0.60
2:B:306:ASN:C	2:B:308:GLU:H	2.09	0.60
2:B:306:ASN:O	2:B:308:GLU:N	2.34	0.60
2:B:395:LYS:HG2	2:B:399:GLU:OE1	2.01	0.60
1:A:108:VAL:HG23	1:A:108:VAL:O	2.02	0.60
2:B:27:THR:HG22	2:B:29:GLU:HB3	1.82	0.60
2:B:308:GLU:C	2:B:310:LEU:N	2.59	0.60
2:B:376:THR:O	2:B:380:ILE:HG13	2.01	0.60
1:A:55:PRO:HB2	1:A:143:ARG:NH2	2.17	0.60
1:A:57:ASN:OD1	1:A:131:THR:HB	2.01	0.60
1:A:503:LEU:CG	1:A:507:GLN:HE22	2.13	0.60
1:A:226:PRO:HG3	1:A:235:HIS:HE1	1.64	0.60
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.67	0.60
2:B:61:PHE:HB3	4:B:1121:HOH:O	2.02	0.59
1:A:3:SER:HB2	1:A:4:PRO:HD2	1.83	0.59
1:A:183:TYR:HE2	1:A:230:MET:SD	2.23	0.59
2:B:224:GLU:HG3	4:B:1151:HOH:O	2.01	0.59
1:A:10:VAL:CG1	1:A:11:LYS:N	2.65	0.59
1:A:134:SER:HB2	1:A:139:THR:OG1	2.02	0.59
1:A:195:ILE:HD11	1:A:199:ARG:CZ	2.32	0.59
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.38	0.59
2:B:419:THR:O	2:B:420:PRO:C	2.42	0.59
1:A:332:GLN:OE1	1:A:338:THR:HG23	2.02	0.59
2:B:105:SER:O	2:B:190:GLY:HA2	2.02	0.59
1:A:242:GLN:O	1:A:243:PRO:C	2.46	0.59
1:A:125:ARG:O	1:A:128:THR:OG1	2.20	0.59
1:A:131:THR:OG1	1:A:143:ARG:HG3	2.01	0.59
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.38	0.59
1:A:503:LEU:CG	1:A:507:GLN:NE2	2.64	0.59
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.83	0.59
2:B:84:THR:O	2:B:86:ASP:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.33	0.58
1:A:507:GLN:C	1:A:509:GLN:H	2.11	0.58
2:B:374:LYS:O	2:B:378:GLU:HG3	2.03	0.58
1:A:17:ASP:O	1:A:83:ARG:HD3	2.03	0.58
1:A:402:TRP:HE3	1:A:402:TRP:O	1.86	0.58
2:B:195:ILE:HD13	2:B:199:ARG:HH21	1.69	0.58
1:A:501:TYR:CD1	1:A:505:ILE:HD11	2.38	0.58
2:B:277:ARG:H	2:B:277:ARG:CD	1.96	0.58
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.68	0.58
2:B:4:PRO:HG3	2:B:117:SER:HB2	1.85	0.58
2:B:27:THR:HG22	2:B:30:LYS:H	1.68	0.58
1:A:173:LYS:O	1:A:176:PRO:HD3	2.04	0.58
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.69	0.58
1:A:182:GLN:HB3	1:A:187:LEU:HD12	1.85	0.57
1:A:253:THR:O	1:A:256:ASP:N	2.35	0.57
2:B:340:GLN:N	2:B:340:GLN:CD	2.62	0.57
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.87	0.57
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.86	0.57
1:A:382:ILE:HG23	2:B:136:ASN:HD21	1.67	0.57
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.85	0.57
1:A:54:ASN:O	1:A:55:PRO:C	2.46	0.57
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.87	0.57
1:A:19:PRO:O	1:A:56:TYR:CB	2.53	0.57
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.70	0.57
1:A:100:LEU:HD21	3:A:701:ADB:CL2	2.41	0.57
1:A:27:THR:O	1:A:28:GLU:C	2.48	0.57
1:A:81:ASN:O	1:A:83:ARG:N	2.38	0.57
2:B:120:LEU:O	2:B:121:ASP:C	2.48	0.57
1:A:100:LEU:HD22	3:A:701:ADB:C8	2.35	0.56
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.40	0.56
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.39	0.56
1:A:460:ASN:H	1:A:460:ASN:ND2	1.94	0.56
1:A:32:LYS:O	1:A:36:GLU:HG3	2.05	0.56
1:A:116:PHE:O	1:A:148:VAL:HG11	2.03	0.56
1:A:356:ARG:NH1	1:A:358:ARG:O	2.38	0.56
1:A:506:ILE:CG2	1:A:507:GLN:N	2.68	0.56
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.88	0.56
2:B:376:THR:HB	2:B:410:TRP:CH2	2.39	0.56
2:B:194:GLU:O	2:B:195:ILE:C	2.49	0.56
2:B:222:GLN:HG2	2:B:223:LYS:N	2.21	0.56
1:A:22:LYS:CG	1:A:24:TRP:CZ2	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:C	1:A:83:ARG:N	2.63	0.56
2:B:5:ILE:CG2	2:B:6:GLU:H	2.11	0.56
2:B:13:LYS:O	2:B:16:MET:HB2	2.04	0.56
1:A:288:ALA:CB	1:A:291:GLU:CB	2.72	0.56
2:B:231:GLY:O	2:B:233:GLU:HG3	2.06	0.56
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.38	0.56
1:A:497:THR:HG22	1:A:498:ASP:H	1.66	0.56
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.37	0.56
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.40	0.56
1:A:433:PRO:CG	2:B:255:ASN:HD22	2.18	0.56
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.06	0.56
1:A:112:GLY:C	1:A:114:ALA:H	2.14	0.56
2:B:225:PRO:C	2:B:227:PHE:H	2.14	0.56
1:A:235:HIS:HB2	1:A:238:LYS:O	2.06	0.56
1:A:402:TRP:CE3	1:A:402:TRP:C	2.84	0.56
2:B:168:LEU:CD1	2:B:180:ILE:HG21	2.35	0.55
2:B:222:GLN:HG2	2:B:223:LYS:H	1.70	0.55
1:A:362:THR:HG22	1:A:363:ASN:N	2.19	0.55
2:B:345:PRO:HB2	2:B:346:PHE:CE1	2.42	0.55
2:B:394:GLN:O	2:B:395:LYS:C	2.48	0.55
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.40	0.55
2:B:98:ALA:O	2:B:101:LYS:HE2	2.07	0.55
2:B:395:LYS:CG	2:B:399:GLU:OE1	2.55	0.55
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.21	0.55
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.70	0.55
2:B:330:GLN:HE21	2:B:338:THR:C	2.14	0.55
1:A:277:ARG:CD	1:A:334:GLN:HB3	2.36	0.55
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.22	0.55
2:B:206:ARG:HB3	2:B:206:ARG:CZ	2.37	0.55
2:B:245:VAL:HG12	2:B:246:LEU:O	2.06	0.55
2:B:306:ASN:C	2:B:308:GLU:N	2.64	0.55
1:A:168:LEU:O	1:A:169:GLU:C	2.48	0.55
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.41	0.55
2:B:146:TYR:CD1	2:B:150:PRO:HB3	2.41	0.55
1:A:434:ILE:N	1:A:494:ASN:HD21	2.04	0.55
1:A:19:PRO:O	1:A:57:ASN:N	2.40	0.55
1:A:388:LYS:HZ2	1:A:413:GLU:HG3	1.71	0.55
1:A:501:TYR:C	1:A:505:ILE:HD12	2.32	0.55
2:B:246:LEU:HD23	2:B:246:LEU:N	2.22	0.55
2:B:301:LEU:O	2:B:305:GLU:HB3	2.07	0.55
1:A:369:THR:CG2	1:A:398:TRP:HH2	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HD11	2:B:233:GLU:OE1	2.06	0.55
1:A:29:GLU:O	1:A:32:LYS:HE2	2.07	0.54
2:B:41:MET:HE3	2:B:116:PHE:HE1	1.71	0.54
2:B:328:GLU:HB3	4:B:1149:HOH:O	2.06	0.54
1:A:175:ASN:HB3	1:A:178:ILE:CD1	2.37	0.54
2:B:78:ARG:HD3	2:B:411:ILE:O	2.07	0.54
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.08	0.54
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.42	0.54
2:B:2:ILE:HG23	2:B:2:ILE:O	2.06	0.54
2:B:345:PRO:C	2:B:346:PHE:CD1	2.86	0.54
1:A:55:PRO:HB2	1:A:143:ARG:CZ	2.36	0.54
1:A:82:LYS:O	1:A:82:LYS:HG2	2.08	0.54
1:A:500:GLN:O	1:A:501:TYR:C	2.50	0.54
1:A:182:GLN:HA	1:A:187:LEU:HA	1.89	0.54
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.42	0.54
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.43	0.54
2:B:206:ARG:NH1	2:B:216:THR:OG1	2.40	0.54
2:B:296:THR:H	2:B:299:ALA:HB3	1.73	0.54
1:A:173:LYS:C	1:A:175:ASN:H	2.16	0.54
1:A:287:LYS:HG2	1:A:288:ALA:N	2.21	0.54
2:B:85:GLN:C	2:B:85:GLN:OE1	2.51	0.54
2:B:73:LYS:HE2	2:B:75:VAL:HG22	1.90	0.54
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.38	0.54
1:A:102:LYS:HG2	1:A:104:LYS:HZ3	1.71	0.54
1:A:215:THR:HG22	1:A:216:THR:N	2.23	0.54
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.43	0.54
1:A:429:LEU:HD11	1:A:506:ILE:CG2	2.38	0.54
2:B:125:ARG:O	2:B:127:TYR:N	2.40	0.54
1:A:139:THR:HB	1:A:140:PRO:CD	2.37	0.53
1:A:315:HIS:CE1	1:A:347:LYS:CD	2.90	0.53
2:B:357:MET:HE3	2:B:361:HIS:CD2	2.42	0.53
1:A:90:VAL:CG1	1:A:91:GLN:HG3	2.33	0.53
2:B:156:SER:H	2:B:157:PRO:HD2	1.72	0.53
2:B:206:ARG:HB3	2:B:206:ARG:HH11	1.70	0.53
1:A:112:GLY:HA2	1:A:185:ASP:OD1	2.09	0.53
1:A:257:ILE:CG2	1:A:283:LEU:HD13	2.38	0.53
1:A:136:ASN:C	1:A:138:GLU:H	2.17	0.53
2:B:276:VAL:O	2:B:279:LEU:N	2.40	0.53
2:B:330:GLN:H	2:B:330:GLN:NE2	2.06	0.53
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.91	0.53
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLU:C	1:A:55:PRO:CD	2.80	0.53
1:A:335:GLY:HA2	1:A:367:GLN:NE2	2.23	0.53
2:B:78:ARG:CZ	2:B:411:ILE:HG21	2.39	0.53
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.43	0.53
1:A:304:ALA:O	1:A:307:ARG:N	2.33	0.53
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.39	0.53
2:B:136:ASN:O	2:B:137:ASN:HB2	2.08	0.53
1:A:183:TYR:C	1:A:184:MET:CG	2.82	0.53
1:A:276:VAL:HG12	1:A:276:VAL:O	2.07	0.53
1:A:362:THR:CG2	1:A:363:ASN:N	2.71	0.53
1:A:28:GLU:HB3	1:A:135:ILE:CD1	2.37	0.53
1:A:54:ASN:N	1:A:55:PRO:HD3	2.24	0.53
1:A:117:SER:CB	1:A:214:LEU:HD23	2.39	0.53
1:A:50:ILE:CG1	1:A:51:GLY:N	2.71	0.52
1:A:297:GLU:HB2	1:A:298:GLU:OE2	2.10	0.52
1:A:191:SER:OG	1:A:198:HIS:ND1	2.38	0.52
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.52
1:A:393:ILE:HG23	1:A:414:TRP:CZ3	2.45	0.52
2:B:11:LYS:HG2	2:B:12:LEU:O	2.10	0.52
2:B:84:THR:O	2:B:87:PHE:N	2.43	0.52
2:B:91:GLN:O	2:B:92:LEU:HD23	2.10	0.52
2:B:220:LYS:HD2	2:B:231:GLY:N	2.25	0.52
2:B:191:SER:OG	2:B:198:HIS:ND1	2.24	0.52
1:A:50:ILE:HG13	1:A:51:GLY:H	1.75	0.52
2:B:161:GLN:O	2:B:162:SER:C	2.53	0.52
2:B:198:HIS:O	2:B:199:ARG:C	2.52	0.52
2:B:344:GLU:O	2:B:345:PRO:C	2.52	0.52
2:B:406:TRP:NE1	2:B:408:ALA:HB3	2.25	0.52
1:A:340:GLN:CB	1:A:351:THR:HG22	2.39	0.52
1:A:19:PRO:O	1:A:56:TYR:HB3	2.10	0.52
1:A:240:THR:HG23	1:A:241:VAL:N	2.24	0.52
1:A:494:ASN:HD22	2:B:289:LEU:HD12	1.74	0.52
1:A:507:GLN:C	1:A:509:GLN:N	2.65	0.52
2:B:314:VAL:HG13	2:B:317:VAL:HG21	1.92	0.52
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.40	0.51
1:A:460:ASN:ND2	1:A:461:LYS:H	2.08	0.51
2:B:57:ASN:HA	2:B:129:ALA:O	2.11	0.51
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.92	0.51
2:B:184:MET:HE3	4:B:1037:HOH:O	2.10	0.51
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.45	0.51
1:A:182:GLN:CD	1:A:182:GLN:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:HD2	1:A:358:ARG:HG3	1.91	0.51
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.92	0.51
1:A:117:SER:HB2	1:A:214:LEU:HD23	1.91	0.51
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.45	0.51
1:A:188:TYR:CD2	3:A:701:ADB:H5	2.45	0.51
1:A:509:GLN:N	1:A:510:PRO:CD	2.73	0.51
1:A:407:GLN:OE1	2:B:394:GLN:N	2.44	0.51
1:A:420:PRO:HA	1:A:421:PRO:O	2.09	0.51
2:B:221:HIS:N	2:B:221:HIS:CD2	2.79	0.51
1:A:277:ARG:HD2	1:A:334:GLN:HB2	1.90	0.51
2:B:242:GLN:HB2	2:B:243:PRO:HD2	1.93	0.51
1:A:287:LYS:HE2	1:A:291:GLU:OE1	2.11	0.51
2:B:2:ILE:O	2:B:3:SER:C	2.54	0.51
1:A:115:TYR:CE2	1:A:151:GLN:HA	2.45	0.51
1:A:229:TRP:O	1:A:232:TYR:N	2.40	0.51
2:B:249:LYS:HD2	2:B:252:TRP:HZ3	1.73	0.51
2:B:296:THR:H	2:B:299:ALA:CB	2.24	0.51
1:A:301:LEU:HD12	1:A:301:LEU:C	2.35	0.51
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.92	0.51
1:A:503:LEU:HD22	1:A:535:TRP:CB	2.31	0.51
1:A:102:LYS:O	1:A:103:LYS:HD3	2.11	0.50
1:A:402:TRP:HE3	1:A:402:TRP:C	2.19	0.50
1:A:424:LYS:HD3	1:A:425:LEU:H	1.73	0.50
1:A:529:GLU:C	1:A:530:LYS:HG3	2.37	0.50
1:A:77:PHE:CE1	1:A:150:PRO:HB3	2.47	0.50
1:A:288:ALA:HB2	1:A:291:GLU:HB2	1.89	0.50
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.77	0.50
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.93	0.50
1:A:3:SER:CB	1:A:4:PRO:HD2	2.41	0.50
2:B:65:LYS:CA	2:B:72:ARG:HG3	2.31	0.50
1:A:13:LYS:CD	1:A:16:MET:HE3	2.39	0.50
1:A:58:THR:HG22	1:A:76:ASP:O	2.12	0.50
1:A:372:VAL:HG11	1:A:411:ILE:HG13	1.94	0.50
1:A:394:GLN:O	1:A:395:LYS:C	2.53	0.50
1:A:417:VAL:HG12	1:A:419:THR:CG2	2.40	0.50
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.42	0.50
1:A:418:ASN:C	1:A:419:THR:HG22	2.37	0.50
2:B:171:PHE:CB	4:B:1153:HOH:O	2.60	0.50
2:B:193:LEU:HD12	2:B:198:HIS:N	2.27	0.50
1:A:504:GLY:O	1:A:505:ILE:C	2.54	0.50
2:B:85:GLN:CG	2:B:154:LYS:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:O	2:B:280:SER:N	2.33	0.50
2:B:306:ASN:HA	2:B:309:ILE:HG22	1.93	0.50
1:A:17:ASP:O	1:A:83:ARG:CD	2.59	0.50
1:A:277:ARG:HH22	1:A:514:GLU:HG3	1.76	0.50
2:B:195:ILE:HD13	2:B:199:ARG:NH2	2.27	0.50
2:B:232:TYR:CE1	2:B:234:LEU:HD21	2.46	0.49
2:B:340:GLN:OE1	2:B:340:GLN:N	2.45	0.49
1:A:162:SER:HB2	2:B:52:PRO:CG	2.42	0.49
2:B:160:PHE:O	2:B:161:GLN:C	2.55	0.49
2:B:326:ILE:CG2	2:B:342:TYR:CE1	2.94	0.49
2:B:411:ILE:HG22	2:B:412:PRO:O	2.12	0.49
1:A:186:ASP:HB3	1:A:188:TYR:HE1	1.76	0.49
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.47	0.49
2:B:27:THR:O	2:B:31:ILE:HD12	2.13	0.49
1:A:96:HIS:CE1	1:A:350:LYS:HE2	2.48	0.49
1:A:203:GLU:O	1:A:206:ARG:HB3	2.13	0.49
2:B:22:LYS:N	2:B:22:LYS:HD2	2.28	0.49
1:A:116:PHE:HE2	1:A:146:TYR:HE1	1.61	0.49
2:B:23:GLN:OE1	2:B:60:VAL:HG22	2.12	0.49
2:B:205:LEU:O	2:B:206:ARG:C	2.54	0.49
2:B:345:PRO:C	2:B:346:PHE:HD1	2.20	0.49
1:A:20:LYS:HA	1:A:57:ASN:H	1.77	0.49
1:A:30:LYS:O	1:A:33:ALA:HB3	2.13	0.49
1:A:253:THR:O	1:A:254:VAL:C	2.56	0.49
1:A:181:TYR:C	1:A:181:TYR:CD2	2.90	0.49
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.95	0.49
1:A:215:THR:HG22	1:A:216:THR:H	1.77	0.49
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.12	0.49
1:A:8:VAL:O	1:A:121:ASP:HB2	2.13	0.48
1:A:57:ASN:ND2	1:A:58:THR:H	2.10	0.48
1:A:104:LYS:HE3	1:A:192:ASP:OD1	2.13	0.48
1:A:343:GLN:HG3	1:A:349:LEU:HD22	1.95	0.48
1:A:376:THR:HG23	1:A:386:THR:CG2	2.41	0.48
1:A:379:SER:HA	1:A:383:TRP:CE3	2.48	0.48
2:B:135:ILE:O	2:B:138:GLU:HG3	2.12	0.48
2:B:220:LYS:HD2	2:B:230:MET:C	2.38	0.48
2:B:373:GLN:NE2	2:B:406:TRP:HA	2.26	0.48
2:B:393:ILE:HG23	2:B:393:ILE:O	2.13	0.48
1:A:182:GLN:H	1:A:182:GLN:NE2	2.10	0.48
1:A:499:SER:OG	1:A:502:ALA:HB3	2.13	0.48
2:B:41:MET:HE3	2:B:116:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:GLU:OE1	2:B:49:LYS:HE3	2.13	0.48
2:B:88:TRP:CB	4:B:1089:HOH:O	2.61	0.48
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.44	0.48
2:B:314:VAL:CG2	2:B:315:HIS:N	2.77	0.48
1:A:22:LYS:HG2	1:A:24:TRP:HZ2	1.70	0.48
1:A:397:THR:O	1:A:398:TRP:C	2.56	0.48
2:B:12:LEU:HD12	2:B:12:LEU:H	1.77	0.48
2:B:246:LEU:HD12	2:B:303:LEU:HD11	1.96	0.48
2:B:325:LEU:HD12	2:B:385:LYS:HG3	1.95	0.48
2:B:411:ILE:C	2:B:412:PRO:O	2.56	0.48
1:A:30:LYS:O	1:A:31:ILE:C	2.56	0.48
1:A:34:LEU:HB2	1:A:132:ILE:HD12	1.96	0.48
1:A:94:ILE:HD13	1:A:230:MET:HE2	1.96	0.48
1:A:229:TRP:O	1:A:232:TYR:HB2	2.13	0.48
1:A:286:THR:O	1:A:286:THR:CG2	2.59	0.48
1:A:9:PRO:O	1:A:9:PRO:HG2	2.14	0.48
1:A:441:TYR:CD2	1:A:542:ILE:HD12	2.48	0.48
1:A:540:LYS:O	1:A:541:GLY:O	2.30	0.48
2:B:246:LEU:HD12	2:B:303:LEU:CD1	2.44	0.48
1:A:30:LYS:C	1:A:33:ALA:H	2.22	0.48
1:A:285:GLY:HA3	1:A:287:LYS:NZ	2.28	0.48
2:B:195:ILE:CD1	2:B:199:ARG:NE	2.77	0.48
2:B:326:ILE:HG21	2:B:342:TYR:CE1	2.47	0.48
2:B:422:LEU:HD12	2:B:425:LEU:CD1	2.40	0.48
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.77	0.48
1:A:369:THR:HG1	1:A:398:TRP:HZ3	1.54	0.48
2:B:60:VAL:HG11	2:B:130:PHE:HD2	1.75	0.48
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.48	0.48
2:B:246:LEU:HD21	2:B:310:LEU:CD1	2.44	0.48
1:A:354:TYR:HA	4:A:1141:HOH:O	2.13	0.48
1:A:58:THR:HG22	1:A:59:PRO:CD	2.40	0.47
2:B:30:LYS:HD3	2:B:71:TRP:CH2	2.49	0.47
2:B:195:ILE:CG2	2:B:196:GLY:N	2.77	0.47
2:B:342:TYR:C	2:B:342:TYR:HD1	2.21	0.47
1:A:53:GLU:N	1:A:55:PRO:HD3	2.29	0.47
2:B:27:THR:HG23	4:B:1003:HOH:O	2.12	0.47
2:B:76:ASP:OD2	2:B:78:ARG:NH2	2.38	0.47
2:B:201:LYS:HA	2:B:201:LYS:HD3	1.65	0.47
2:B:283:LEU:C	2:B:285:GLY:N	2.72	0.47
1:A:240:THR:HG23	1:A:241:VAL:O	2.14	0.47
1:A:326:ILE:CD1	1:A:343:GLN:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ILE:O	1:A:525:LEU:HB2	2.14	0.47
2:B:40:GLU:O	2:B:41:MET:C	2.54	0.47
1:A:20:LYS:HG2	1:A:56:TYR:HA	1.96	0.47
1:A:223:LYS:H	1:A:223:LYS:CD	2.27	0.47
2:B:27:THR:O	2:B:28:GLU:C	2.56	0.47
2:B:168:LEU:C	2:B:170:PRO:HD2	2.40	0.47
1:A:427:TYR:CD1	1:A:427:TYR:C	2.93	0.47
2:B:90:VAL:O	2:B:91:GLN:C	2.57	0.47
1:A:56:TYR:H	1:A:56:TYR:HD1	1.58	0.47
1:A:64:LYS:CE	1:A:68:SER:CB	2.91	0.47
1:A:294:PRO:O	1:A:295:LEU:C	2.57	0.47
2:B:23:GLN:HG3	2:B:23:GLN:O	2.15	0.47
2:B:298:GLU:O	2:B:301:LEU:CB	2.62	0.47
1:A:369:THR:HG23	1:A:398:TRP:HH2	1.79	0.47
2:B:30:LYS:O	2:B:31:ILE:C	2.57	0.47
2:B:232:TYR:HE1	2:B:234:LEU:HD21	1.80	0.47
1:A:258:GLN:HG2	1:A:283:LEU:CD2	2.44	0.47
2:B:280:SER:O	2:B:281:LYS:C	2.58	0.47
2:B:346:PHE:CD1	2:B:346:PHE:N	2.82	0.47
2:B:419:THR:O	2:B:421:PRO:N	2.48	0.47
1:A:96:HIS:CE1	1:A:269:GLN:HE21	2.33	0.46
1:A:135:ILE:O	1:A:135:ILE:HG13	2.12	0.46
1:A:254:VAL:HA	1:A:257:ILE:HG22	1.97	0.46
1:A:278:GLN:HG2	1:A:302:GLU:OE2	2.15	0.46
1:A:410:TRP:HB2	2:B:365:VAL:HG21	1.97	0.46
1:A:344:GLU:HA	1:A:345:PRO:HD3	1.66	0.46
2:B:305:GLU:O	2:B:308:GLU:HB3	2.16	0.46
1:A:279:LEU:HD23	1:A:299:ALA:CB	2.34	0.46
2:B:85:GLN:HB2	2:B:154:LYS:HB2	1.95	0.46
2:B:375:ILE:HB	2:B:389:PHE:HZ	1.80	0.46
1:A:173:LYS:O	1:A:175:ASN:N	2.48	0.46
1:A:457:TYR:C	1:A:457:TYR:CD2	2.93	0.46
2:B:11:LYS:NZ	2:B:14:PRO:HG3	2.31	0.46
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.95	0.46
1:A:24:TRP:N	1:A:25:PRO:CD	2.79	0.46
1:A:308:GLU:O	1:A:312:GLU:OE1	2.33	0.46
3:A:701:ADB:H16	3:A:701:ADB:N1	2.31	0.46
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.46
2:B:277:ARG:HA	2:B:280:SER:OG	2.16	0.46
2:B:411:ILE:O	2:B:412:PRO:O	2.34	0.46
1:A:329:ILE:HA	1:A:338:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LYS:HG3	1:A:541:GLY:N	2.31	0.46
2:B:246:LEU:HD21	2:B:310:LEU:HD13	1.98	0.46
1:A:3:SER:HB3	1:A:212:TRP:O	2.15	0.46
1:A:170:PRO:HG2	1:A:171:PHE:H	1.80	0.46
1:A:331:LYS:HZ3	1:A:333:GLY:HA2	1.80	0.46
1:A:398:TRP:O	1:A:399:GLU:C	2.59	0.46
1:A:506:ILE:HD11	1:A:521:ILE:HG21	1.97	0.46
2:B:84:THR:O	2:B:85:GLN:C	2.59	0.46
2:B:169:GLU:N	2:B:170:PRO:HD2	2.30	0.46
2:B:195:ILE:O	2:B:196:GLY:C	2.59	0.46
2:B:222:GLN:CG	2:B:223:LYS:H	2.29	0.46
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.98	0.46
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.82	0.46
2:B:115:TYR:O	2:B:117:SER:N	2.49	0.46
1:A:244:ILE:CD1	1:A:310:LEU:HD13	2.19	0.45
1:A:288:ALA:HB1	1:A:291:GLU:H	1.81	0.45
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.80	0.45
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.49	0.45
1:A:85:GLN:HE22	2:B:53:GLU:HB2	1.81	0.45
1:A:426:TRP:O	1:A:427:TYR:HB3	2.16	0.45
1:A:429:LEU:HD11	1:A:506:ILE:HG23	1.98	0.45
1:A:497:THR:CG2	1:A:498:ASP:H	2.27	0.45
2:B:319:TYR:O	2:B:321:PRO:HD3	2.17	0.45
1:A:120:LEU:O	1:A:122:GLU:N	2.49	0.45
1:A:298:GLU:O	1:A:299:ALA:C	2.59	0.45
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.29	0.45
1:A:104:LYS:CE	1:A:192:ASP:OD1	2.64	0.45
1:A:356:ARG:HG2	1:A:367:GLN:HG3	1.98	0.45
2:B:139:THR:HG23	2:B:140:PRO:CD	2.44	0.45
1:A:53:GLU:H	1:A:55:PRO:HD3	1.80	0.45
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.99	0.45
1:A:379:SER:CB	1:A:387:PRO:HD3	2.47	0.45
1:A:398:TRP:O	1:A:400:THR:N	2.49	0.45
1:A:474:ASN:C	1:A:478:GLU:HG3	2.40	0.45
2:B:164:MET:O	2:B:165:THR:C	2.58	0.45
1:A:18:GLY:HA2	1:A:19:PRO:HD3	1.84	0.45
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.52	0.45
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.69	0.45
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.51	0.45
2:B:46:LYS:HD3	2:B:116:PHE:CE1	2.52	0.45
2:B:202:ILE:O	2:B:205:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:HIS:O	2:B:201:LYS:N	2.50	0.45
2:B:324:ASP:O	2:B:343:GLN:HG2	2.17	0.45
2:B:363:ASN:ND2	2:B:365:VAL:N	2.65	0.45
1:A:410:TRP:HB2	2:B:365:VAL:CG2	2.46	0.45
1:A:513:SER:O	1:A:519:ASN:ND2	2.50	0.45
2:B:153:TRP:O	2:B:155:GLY:N	2.48	0.45
1:A:309:ILE:O	1:A:312:GLU:CD	2.60	0.44
2:B:115:TYR:C	2:B:117:SER:H	2.25	0.44
2:B:171:PHE:HB3	4:B:1153:HOH:O	2.15	0.44
1:A:395:LYS:HE2	1:A:399:GLU:OE1	2.16	0.44
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.47	0.44
2:B:267:ALA:O	2:B:269:GLN:N	2.51	0.44
2:B:274:ILE:HG22	2:B:275:LYS:N	2.32	0.44
1:A:126:LYS:HE2	1:A:126:LYS:HB3	1.69	0.44
1:A:369:THR:HG23	1:A:398:TRP:CH2	2.53	0.44
2:B:135:ILE:C	2:B:137:ASN:H	2.24	0.44
2:B:209:LEU:HD22	2:B:214:LEU:HD12	1.99	0.44
2:B:257:ILE:HD11	2:B:279:LEU:O	2.18	0.44
2:B:339:TYR:CG	2:B:375:ILE:HD13	2.52	0.44
1:A:60:VAL:HG22	1:A:130:PHE:HB2	2.00	0.44
1:A:169:GLU:O	1:A:170:PRO:C	2.59	0.44
1:A:379:SER:O	1:A:380:ILE:C	2.60	0.44
1:A:412:PRO:O	1:A:414:TRP:HD1	2.01	0.44
1:A:474:ASN:O	1:A:475:GLN:C	2.58	0.44
1:A:521:ILE:O	1:A:522:ILE:C	2.59	0.44
2:B:163:SER:O	2:B:167:ILE:HG13	2.17	0.44
2:B:363:ASN:HD22	2:B:364:ASP:N	2.08	0.44
2:B:366:LYS:O	2:B:370:GLU:HG3	2.18	0.44
1:A:184:MET:HE3	1:A:184:MET:HB3	1.70	0.44
1:A:253:THR:O	1:A:256:ASP:HB2	2.18	0.44
1:A:499:SER:OG	1:A:502:ALA:CB	2.66	0.44
2:B:153:TRP:C	2:B:155:GLY:H	2.25	0.44
1:A:37:ILE:O	1:A:41:MET:HB2	2.18	0.44
1:A:411:ILE:HG13	1:A:412:PRO:HD2	2.00	0.44
1:A:418:ASN:C	1:A:419:THR:CG2	2.91	0.44
1:A:424:LYS:HD3	1:A:425:LEU:C	2.43	0.44
1:A:435:VAL:HA	2:B:290:THR:OG1	2.18	0.44
1:A:504:GLY:O	1:A:507:GLN:N	2.50	0.44
2:B:139:THR:HG22	2:B:140:PRO:O	2.17	0.44
2:B:234:LEU:HD11	2:B:377:THR:HG21	1.99	0.44
2:B:275:LYS:HB2	2:B:302:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:O	1:A:84:THR:HG23	2.17	0.44
1:A:231:GLY:O	1:A:242:GLN:HG2	2.18	0.44
1:A:388:LYS:NZ	4:A:1155:HOH:O	2.28	0.44
2:B:276:VAL:O	2:B:277:ARG:C	2.61	0.44
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.87	0.44
1:A:104:LYS:N	1:A:104:LYS:CE	2.75	0.44
1:A:129:ALA:HA	1:A:144:TYR:O	2.17	0.44
1:A:158:ALA:C	1:A:160:PHE:N	2.75	0.44
1:A:320:ASP:OD2	1:A:322:SER:OG	2.36	0.44
1:A:330:GLN:HE21	1:A:330:GLN:HB3	1.61	0.44
1:A:354:TYR:CZ	1:A:370:GLU:HB3	2.53	0.44
2:B:104:LYS:O	2:B:105:SER:OG	2.34	0.44
2:B:109:LEU:HA	2:B:218:ASP:OD2	2.18	0.44
2:B:156:SER:O	2:B:157:PRO:C	2.61	0.44
2:B:259:LYS:O	2:B:262:GLY:N	2.50	0.44
1:A:51:GLY:O	1:A:53:GLU:N	2.51	0.43
1:A:112:GLY:C	1:A:114:ALA:N	2.76	0.43
1:A:173:LYS:C	1:A:175:ASN:N	2.75	0.43
1:A:235:HIS:HB2	1:A:238:LYS:HG2	2.00	0.43
1:A:288:ALA:HB3	1:A:291:GLU:HB3	1.95	0.43
2:B:33:ALA:O	2:B:37:ILE:HG13	2.18	0.43
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.80	0.43
2:B:278:GLN:CD	2:B:298:GLU:H	2.26	0.43
1:A:241:VAL:HG12	1:A:242:GLN:N	2.33	0.43
2:B:27:THR:HG21	2:B:29:GLU:HB3	1.99	0.43
2:B:255:ASN:O	2:B:258:GLN:N	2.50	0.43
2:B:330:GLN:N	2:B:330:GLN:CD	2.76	0.43
2:B:395:LYS:HE2	2:B:399:GLU:OE2	2.18	0.43
1:A:57:ASN:ND2	1:A:58:THR:N	2.66	0.43
1:A:390:LYS:HB3	1:A:417:VAL:HG21	2.00	0.43
2:B:30:LYS:HD2	2:B:62:ALA:HB3	2.01	0.43
2:B:267:ALA:C	2:B:269:GLN:H	2.27	0.43
2:B:375:ILE:HD12	2:B:389:PHE:HE2	1.82	0.43
2:B:296:THR:O	2:B:297:GLU:C	2.60	0.43
1:A:328:GLU:HG3	1:A:390:LYS:CB	2.34	0.43
1:A:342:TYR:HA	1:A:349:LEU:HB2	2.01	0.43
2:B:13:LYS:O	2:B:16:MET:CB	2.64	0.43
2:B:27:THR:HB	2:B:30:LYS:CG	2.49	0.43
2:B:46:LYS:HZ3	2:B:116:PHE:HD1	1.66	0.43
2:B:85:GLN:CB	2:B:154:LYS:HB2	2.49	0.43
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:O	2:B:198:HIS:HB3	2.19	0.43
2:B:266:TRP:CD1	2:B:422:LEU:HD23	2.53	0.43
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.79	0.43
1:A:331:LYS:HZ1	1:A:333:GLY:HA2	1.81	0.43
2:B:34:LEU:O	2:B:35:VAL:C	2.58	0.43
2:B:64:LYS:O	2:B:65:LYS:C	2.61	0.43
1:A:136:ASN:C	1:A:138:GLU:N	2.76	0.43
1:A:229:TRP:NE1	1:A:230:MET:HG2	2.33	0.43
1:A:300:GLU:O	1:A:301:LEU:C	2.61	0.43
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.30	0.43
2:B:303:LEU:HD22	4:B:1143:HOH:O	2.19	0.43
2:B:308:GLU:O	2:B:310:LEU:N	2.51	0.43
2:B:195:ILE:HG12	2:B:199:ARG:HG3	2.01	0.43
1:A:395:LYS:O	1:A:396:GLU:C	2.62	0.43
1:A:531:VAL:HG12	1:A:532:TYR:N	2.33	0.43
2:B:203:GLU:HA	2:B:206:ARG:HB2	2.01	0.43
2:B:257:ILE:HG23	2:B:258:GLN:N	2.33	0.43
2:B:278:GLN:CA	2:B:281:LYS:HE3	2.22	0.43
2:B:312:GLU:O	2:B:313:PRO:C	2.61	0.43
1:A:30:LYS:HA	1:A:33:ALA:CB	2.49	0.43
1:A:328:GLU:CG	1:A:390:LYS:HB2	2.36	0.43
2:B:283:LEU:O	2:B:285:GLY:N	2.51	0.43
1:A:91:GLN:C	1:A:93:GLY:N	2.76	0.42
1:A:128:THR:HB	1:A:146:TYR:HB2	2.01	0.42
1:A:137:ASN:O	1:A:138:GLU:HB3	2.18	0.42
1:A:257:ILE:HG21	1:A:283:LEU:HD13	2.01	0.42
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.70	0.42
1:A:491:LEU:HB3	1:A:529:GLU:HB2	2.00	0.42
2:B:329:ILE:N	4:B:1149:HOH:O	2.51	0.42
1:A:64:LYS:HD3	1:A:71:TRP:CH2	2.54	0.42
1:A:294:PRO:O	1:A:296:THR:N	2.53	0.42
1:A:424:LYS:CD	1:A:425:LEU:N	2.79	0.42
2:B:115:TYR:OH	2:B:184:MET:O	2.37	0.42
2:B:125:ARG:C	2:B:127:TYR:N	2.77	0.42
2:B:199:ARG:O	2:B:202:ILE:HB	2.19	0.42
1:A:62:ALA:HB1	1:A:71:TRP:CD1	2.54	0.42
1:A:195:ILE:O	1:A:199:ARG:HG3	2.19	0.42
2:B:16:MET:HE3	2:B:16:MET:HA	2.00	0.42
2:B:236:PRO:HA	2:B:239:TRP:CG	2.53	0.42
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.54	0.42
1:A:203:GLU:O	1:A:204:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CH2	1:A:407:GLN:HG3	2.54	0.42
2:B:13:LYS:HG2	2:B:14:PRO:O	2.20	0.42
2:B:40:GLU:O	2:B:43:LYS:N	2.52	0.42
2:B:124:PHE:O	2:B:125:ARG:C	2.62	0.42
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.55	0.42
2:B:314:VAL:HG22	2:B:315:HIS:N	2.34	0.42
2:B:330:GLN:NE2	2:B:338:THR:C	2.77	0.42
1:A:34:LEU:HB2	1:A:132:ILE:CD1	2.49	0.42
1:A:470:THR:O	1:A:471:ASN:CB	2.67	0.42
1:A:19:PRO:HG2	1:A:80:LEU:HB2	2.01	0.42
2:B:195:ILE:HG23	2:B:196:GLY:H	1.81	0.42
2:B:200:THR:C	2:B:202:ILE:N	2.76	0.42
2:B:222:GLN:CG	2:B:223:LYS:N	2.83	0.42
1:A:341:ILE:O	1:A:349:LEU:HB3	2.20	0.42
1:A:94:ILE:CD1	1:A:230:MET:HE2	2.50	0.42
1:A:160:PHE:O	1:A:161:GLN:C	2.63	0.42
1:A:542:ILE:HD13	1:A:544:GLY:CA	2.50	0.42
2:B:86:ASP:C	2:B:88:TRP:H	2.28	0.42
2:B:302:GLU:O	2:B:306:ASN:HB2	2.19	0.42
1:A:5:ILE:HD11	1:A:167:ILE:HD11	2.01	0.42
1:A:59:PRO:O	1:A:75:VAL:HA	2.20	0.42
1:A:97:PRO:CG	1:A:232:TYR:CE2	2.99	0.42
2:B:234:LEU:HD11	2:B:377:THR:CG2	2.50	0.42
2:B:327:ALA:HA	4:B:1124:HOH:O	2.20	0.42
1:A:19:PRO:C	1:A:56:TYR:HB3	2.45	0.42
1:A:34:LEU:CB	1:A:132:ILE:HD12	2.50	0.42
1:A:184:MET:C	1:A:186:ASP:H	2.28	0.42
2:B:58:THR:N	4:B:1111:HOH:O	2.53	0.42
2:B:207:GLN:HE21	2:B:207:GLN:HB2	1.55	0.42
2:B:257:ILE:HD12	2:B:282:LEU:HD23	2.01	0.42
2:B:361:HIS:N	2:B:361:HIS:ND1	2.68	0.42
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.20	0.41
1:A:22:LYS:HB3	1:A:24:TRP:CE2	2.55	0.41
1:A:120:LEU:O	1:A:121:ASP:C	2.62	0.41
2:B:57:ASN:C	4:B:1111:HOH:O	2.63	0.41
2:B:171:PHE:C	2:B:173:LYS:N	2.78	0.41
2:B:406:TRP:CE2	2:B:408:ALA:HB3	2.55	0.41
1:A:224:GLU:CB	1:A:225:PRO:CD	2.78	0.41
1:A:257:ILE:HD11	1:A:282:LEU:HB2	2.02	0.41
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.50	0.41
2:B:393:ILE:HD13	2:B:398:TRP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:C	1:A:154:LYS:HZ3	2.29	0.41
1:A:198:HIS:O	1:A:202:ILE:HG12	2.20	0.41
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.34	0.41
1:A:276:VAL:HG12	1:A:280:SER:OG	2.19	0.41
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.78	0.41
1:A:328:GLU:O	1:A:339:TYR:HA	2.20	0.41
1:A:434:ILE:O	1:A:437:ALA:HB3	2.21	0.41
2:B:12:LEU:HD11	2:B:127:TYR:CE2	2.56	0.41
2:B:46:LYS:CD	2:B:116:PHE:CD1	3.01	0.41
2:B:356:ARG:HB2	2:B:367:GLN:HG2	2.01	0.41
1:A:73:LYS:NZ	1:A:130:PHE:CZ	2.79	0.41
1:A:275:LYS:C	1:A:276:VAL:HG23	2.46	0.41
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.55	0.41
2:B:254:VAL:O	2:B:257:ILE:HG23	2.20	0.41
2:B:419:THR:H	2:B:420:PRO:CD	2.33	0.41
1:A:102:LYS:HA	1:A:318:TYR:HD1	1.85	0.41
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.35	0.41
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.85	0.41
2:B:28:GLU:O	2:B:29:GLU:C	2.63	0.41
2:B:46:LYS:CD	2:B:116:PHE:HD1	2.33	0.41
1:A:11:LYS:HB2	1:A:85:GLN:OE1	2.21	0.41
1:A:59:PRO:HD2	1:A:76:ASP:O	2.21	0.41
1:A:195:ILE:HG23	1:A:196:GLY:N	2.34	0.41
2:B:56:TYR:O	2:B:57:ASN:HB2	2.21	0.41
2:B:88:TRP:HB2	4:B:1089:HOH:O	2.20	0.41
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.35	0.41
1:A:104:LYS:CG	1:A:192:ASP:HA	2.42	0.41
1:A:275:LYS:NZ	1:A:332:GLN:HE21	2.18	0.41
1:A:470:THR:O	1:A:471:ASN:HB3	2.20	0.41
1:A:542:ILE:CG1	1:A:543:GLY:N	2.79	0.41
2:B:282:LEU:HG	2:B:293:ILE:CD1	2.35	0.41
2:B:298:GLU:CA	2:B:301:LEU:HB2	2.51	0.41
1:A:108:VAL:O	1:A:108:VAL:CG2	2.68	0.41
1:A:215:THR:O	1:A:216:THR:HG22	2.21	0.41
1:A:410:TRP:HE3	1:A:410:TRP:HA	1.85	0.41
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.56	0.41
2:B:43:LYS:C	2:B:45:GLY:N	2.79	0.41
2:B:52:PRO:C	2:B:54:ASN:H	2.29	0.41
2:B:277:ARG:N	2:B:277:ARG:CD	2.70	0.41
2:B:336:GLN:HG2	2:B:355:ALA:HB2	2.03	0.41
1:A:3:SER:HB2	1:A:5:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:H	1:A:178:ILE:HG13	1.62	0.41
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.55	0.41
2:B:414:TRP:CD1	2:B:414:TRP:C	2.99	0.41
1:A:156:SER:O	1:A:157:PRO:C	2.61	0.40
1:A:252:TRP:CD1	1:A:295:LEU:HD13	2.56	0.40
1:A:281:LYS:HE3	4:A:1074:HOH:O	2.19	0.40
1:A:417:VAL:CG1	1:A:419:THR:CG2	3.00	0.40
1:A:503:LEU:O	1:A:504:GLY:C	2.65	0.40
2:B:224:GLU:HA	2:B:225:PRO:HD3	1.67	0.40
1:A:97:PRO:C	1:A:99:GLY:N	2.77	0.40
1:A:382:ILE:HG22	1:A:383:TRP:CD1	2.57	0.40
2:B:220:LYS:HD3	2:B:229:TRP:O	2.21	0.40
1:A:131:THR:O	1:A:131:THR:CG2	2.70	0.40
2:B:156:SER:N	2:B:157:PRO:CD	2.82	0.40
2:B:382:ILE:O	2:B:382:ILE:CG2	2.67	0.40
1:A:132:ILE:CG2	1:A:142:ILE:O	2.69	0.40
1:A:259:LYS:O	1:A:263:LYS:HG3	2.22	0.40
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.51	0.40
2:B:249:LYS:HB2	2:B:252:TRP:CH2	2.56	0.40
1:A:235:HIS:CB	1:A:238:LYS:HG2	2.52	0.40
2:B:46:LYS:NZ	2:B:116:PHE:HD1	2.19	0.40
2:B:166:LYS:O	2:B:167:ILE:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/560 (98%)	429 (78%)	84 (15%)	37 (7%)	1	1
2	B	425/430 (99%)	327 (77%)	68 (16%)	30 (7%)	1	1
All	All	975/990 (98%)	756 (78%)	152 (16%)	67 (7%)	1	1

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	28	GLU
1	A	54	ASN
1	A	122	GLU
1	A	135	ILE
1	A	137	ASN
1	A	153	TRP
1	A	195	ILE
1	A	412	PRO
1	A	538	ALA
1	A	539	HIS
1	A	541	GLY
2	B	7	THR
2	B	77	PHE
2	B	85	GLN
2	B	116	PHE
2	B	218	ASP
2	B	295	LEU
2	B	360	ALA
2	B	419	THR
1	A	16	MET
1	A	82	LYS
1	A	89	GLU
1	A	121	ASP
1	A	174	GLN
1	A	224	GLU
1	A	276	VAL
1	A	398	TRP
1	A	505	ILE
1	A	516	GLU
2	B	126	LYS
2	B	154	LYS
2	B	220	LYS
2	B	288	ALA
2	B	297	GLU
2	B	307	ARG
2	B	421	PRO
1	A	52	PRO
1	A	213	GLY
1	A	254	VAL
2	B	68	SER
2	B	223	LYS

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Mol	Chain	Res	Type
2	B	232	TYR
2	B	268	SER
1	A	23	GLN
1	A	98	ALA
1	A	162	SER
1	A	237	ASP
1	A	397	THR
1	A	501	TYR
1	A	542	ILE
2	B	18	GLY
2	B	231	GLY
2	B	284	ARG
2	B	345	PRO
1	A	399	GLU
2	B	65	LYS
2	B	91	GLN
2	B	198	HIS
2	B	359	GLY
1	A	69	THR
2	B	420	PRO
1	A	504	GLY
2	B	313	PRO
1	A	169	GLU
2	B	3	SER
1	A	24	TRP

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	494/500 (99%)	443 (90%)	51 (10%)	7	15
2	B	389/392 (99%)	344 (88%)	45 (12%)	5	11
All	All	883/892 (99%)	787 (89%)	96 (11%)	6	13

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	28	GLU
1	A	32	LYS
1	A	40	GLU
1	A	58	THR
1	A	60	VAL
1	A	89	GLU
1	A	91	GLN
1	A	107	THR
1	A	128	THR
1	A	131	THR
1	A	132	ILE
1	A	135	ILE
1	A	161	GLN
1	A	165	THR
1	A	178	ILE
1	A	184	MET
1	A	188	TYR
1	A	216	THR
1	A	217	PRO
1	A	220	LYS
1	A	228	LEU
1	A	244	ILE
1	A	274	ILE
1	A	296	THR
1	A	317	VAL
1	A	326	ILE
1	A	330	GLN
1	A	347	LYS
1	A	349	LEU
1	A	356	ARG
1	A	358	ARG
1	A	364	ASP
1	A	369	THR
1	A	386	THR
1	A	391	LEU
1	A	402	TRP
1	A	403	THR
1	A	407	GLN
1	A	410	TRP
1	A	419	THR
1	A	435	VAL
1	A	450	THR

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Mol	Chain	Res	Type
1	A	460	ASN
1	A	465	LYS
1	A	479	LEU
1	A	496	VAL
1	A	506	ILE
1	A	511	ASP
1	A	536	VAL
1	A	542	ILE
2	B	7	THR
2	B	12	LEU
2	B	22	LYS
2	B	27	THR
2	B	36	GLU
2	B	50	ILE
2	B	67	ASP
2	B	69	THR
2	B	91	GLN
2	B	109	LEU
2	B	113	ASP
2	B	163	SER
2	B	165	THR
2	B	169	GLU
2	B	170	PRO
2	B	177	ASP
2	B	187	LEU
2	B	193	LEU
2	B	194	GLU
2	B	200	THR
2	B	206	ARG
2	B	221	HIS
2	B	239	TRP
2	B	244	ILE
2	B	246	LEU
2	B	277	ARG
2	B	279	LEU
2	B	293	ILE
2	B	301	LEU
2	B	305	GLU
2	B	314	VAL
2	B	317	VAL
2	B	338	THR
2	B	340	GLN

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Mol	Chain	Res	Type
2	B	363	ASN
2	B	366	LYS
2	B	372	VAL
2	B	374	LYS
2	B	375	ILE
2	B	393	ILE
2	B	399	GLU
2	B	403	THR
2	B	411	ILE
2	B	418	ASN
2	B	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	91	GLN
1	A	96	HIS
1	A	151	GLN
1	A	161	GLN
1	A	182	GLN
1	A	235	HIS
1	A	269	GLN
1	A	332	GLN
1	A	361	HIS
1	A	367	GLN
1	A	447	ASN
1	A	460	ASN
1	A	474	ASN
1	A	475	GLN
1	A	487	GLN
1	A	494	ASN
1	A	507	GLN
1	A	509	GLN
1	A	519	ASN
1	A	520	GLN
2	B	174	GLN
2	B	182	GLN
2	B	207	GLN
2	B	222	GLN
2	B	255	ASN
2	B	258	GLN

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Mol	Chain	Res	Type
2	B	265	ASN
2	B	269	GLN
2	B	330	GLN
2	B	340	GLN
2	B	343	GLN
2	B	363	ASN
2	B	394	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	ADB	A	701	-	27,27,27	1.90	8 (29%)	36,37,37	2.45	9 (25%)

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	ADB	A	701	-	-	0/10/10/10	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ADB	C16-C11	4.22	1.46	1.39
3	A	701	ADB	C10-N4	3.71	1.41	1.33
3	A	701	ADB	C16-C15	3.11	1.43	1.38
3	A	701	ADB	C13-C12	2.85	1.43	1.38
3	A	701	ADB	C4-C5	2.65	1.43	1.38
3	A	701	ADB	C1-C2	2.35	1.45	1.41
3	A	701	ADB	C4-C3	2.32	1.42	1.38
3	A	701	ADB	C1-C6	2.29	1.45	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ADB	C8-N1-C9	9.34	120.49	112.86
3	A	701	ADB	N2-C9-N1	-4.75	118.48	126.26
3	A	701	ADB	C10-N2-C9	4.44	121.14	113.77
3	A	701	ADB	C8-O7-C1	4.41	124.56	117.16
3	A	701	ADB	N3-C10-N2	-3.70	119.80	125.48
3	A	701	ADB	N3-C8-N1	-3.46	121.37	127.65
3	A	701	ADB	C1-C6-CL6	2.84	122.14	118.40
3	A	701	ADB	C1-C2-CL2	2.68	121.94	118.40
3	A	701	ADB	N4-C10-N2	2.23	120.57	117.22

There are no chirality outliers.

There are no torsion outliers.

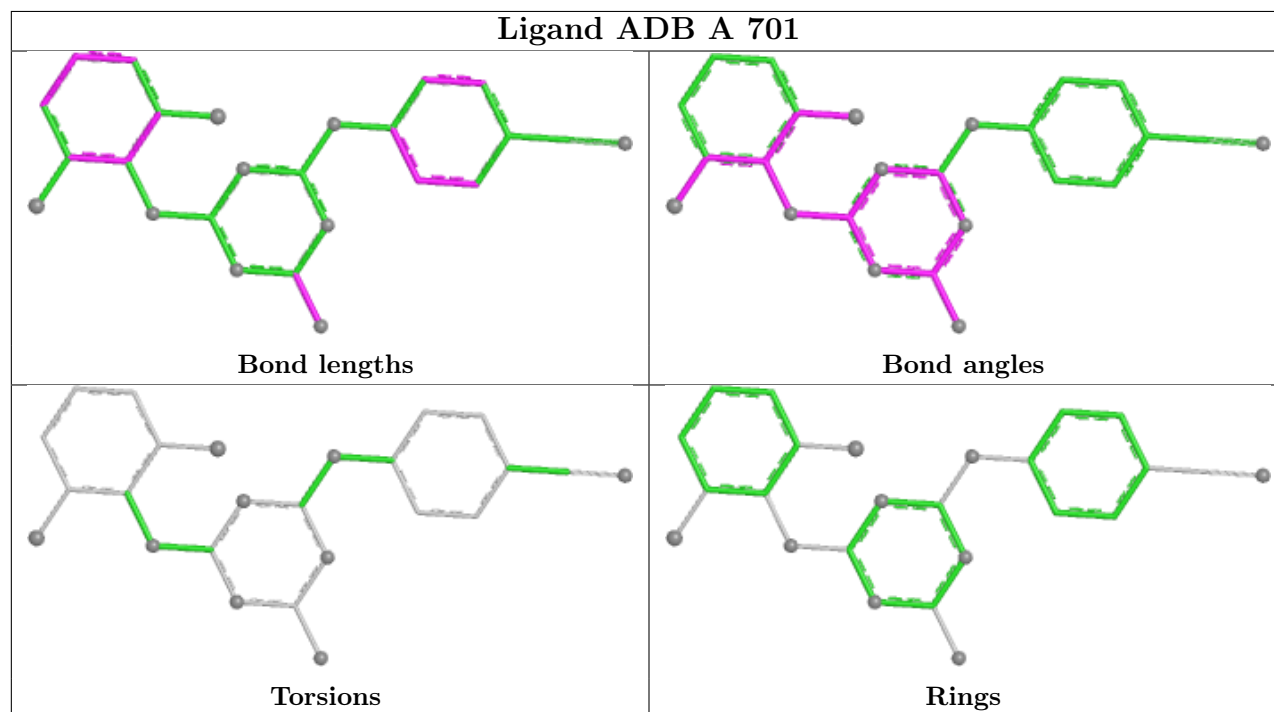
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	ADB	4	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	545/560 (97%)	0.00	10 (1%) 67 63	25, 73, 98, 105	19 (3%)
2	B	427/430 (99%)	-0.06	17 (3%) 42 37	17, 60, 101, 106	14 (3%)
All	All	972/990 (98%)	-0.03	27 (2%) 55 49	17, 69, 100, 106	33 (3%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	4.3
1	A	545	ASN	3.6
2	B	1	PRO	3.5
2	B	360	ALA	3.4
2	B	5	ILE	3.2
2	B	3	SER	3.1
2	B	4	PRO	3.0
2	B	2	ILE	3.0
1	A	21	VAL	3.0
1	A	141	GLY	2.8
2	B	309	ILE	2.8
2	B	232	TYR	2.6
2	B	218	ASP	2.6
2	B	225	PRO	2.5
2	B	304	ALA	2.5
1	A	3	SER	2.5
1	A	544	GLY	2.5
1	A	140	PRO	2.5
2	B	426	TRP	2.4
2	B	427	TYR	2.4
1	A	221	HIS	2.3
1	A	78	ARG	2.3
2	B	230	MET	2.3
1	A	31	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	242	GLN	2.2
1	A	1	PRO	2.1
2	B	295	LEU	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](#)

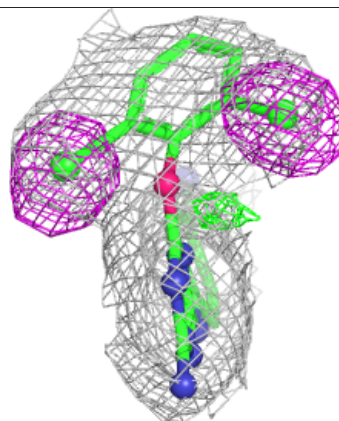
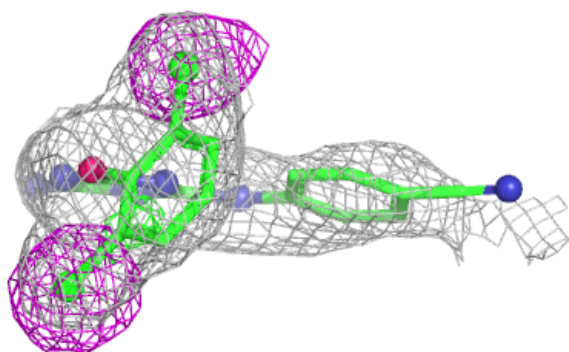
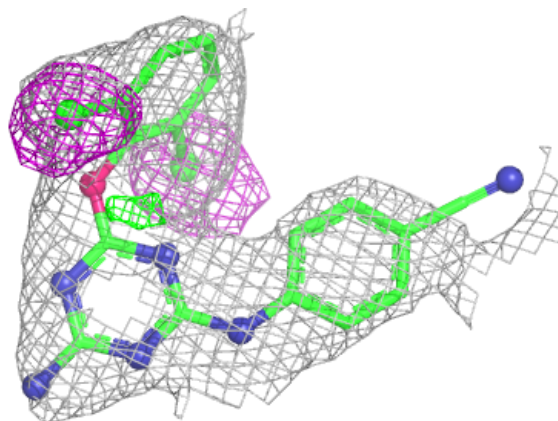
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ADB	A	701	25/25	0.84	0.13	41,56,65,73	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.

Electron density around ADB A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.