



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:15 PM UTC

PDB ID : 1S1V / pdb_00001s1v
Title : Crystal structure of L100I mutant HIV-1 reverse transcriptase in complex with TNK-651
Authors : Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Stammers, D.K.
Deposited on : 2004-01-07
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

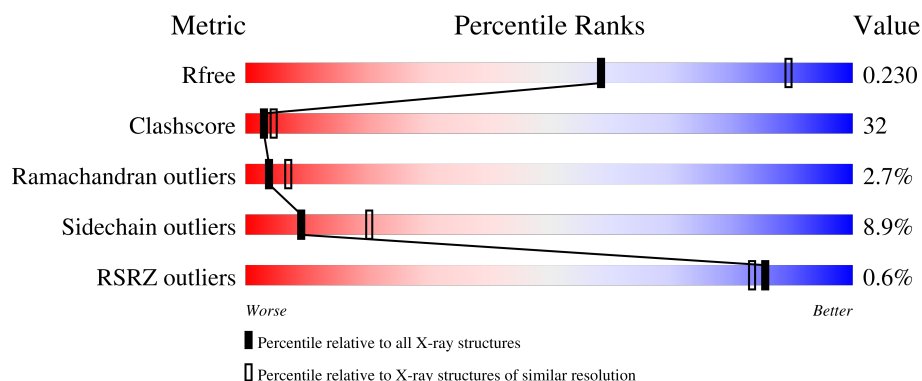
1 Overall quality at a glance

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	% 38% 48% 9% • 5%
2	B	440	 40% 44% 8% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7803 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 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4370	2830	727	805	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ILE	LEU	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

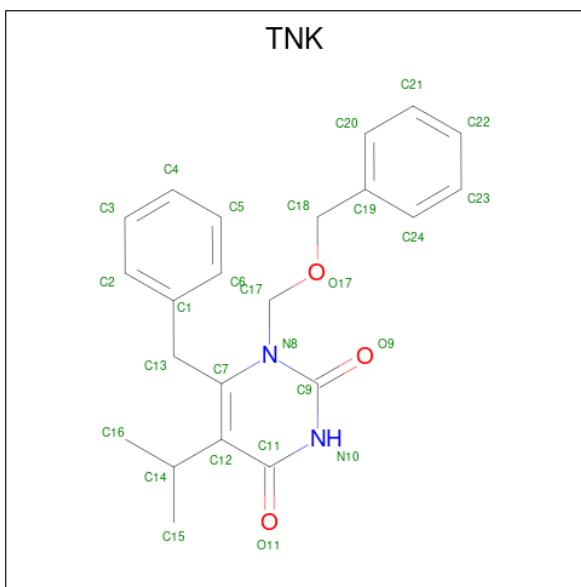
- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3339	2172	555	605	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ILE	LEU	engineered mutation	UNP P04585

- Molecule 3 is 6-BENZYL-1-BENZYLOXYMETHYL-5-ISOPROPYL URACIL (CCD ID: TNK) (formula: C₂₂H₂₄N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	22	2	3		

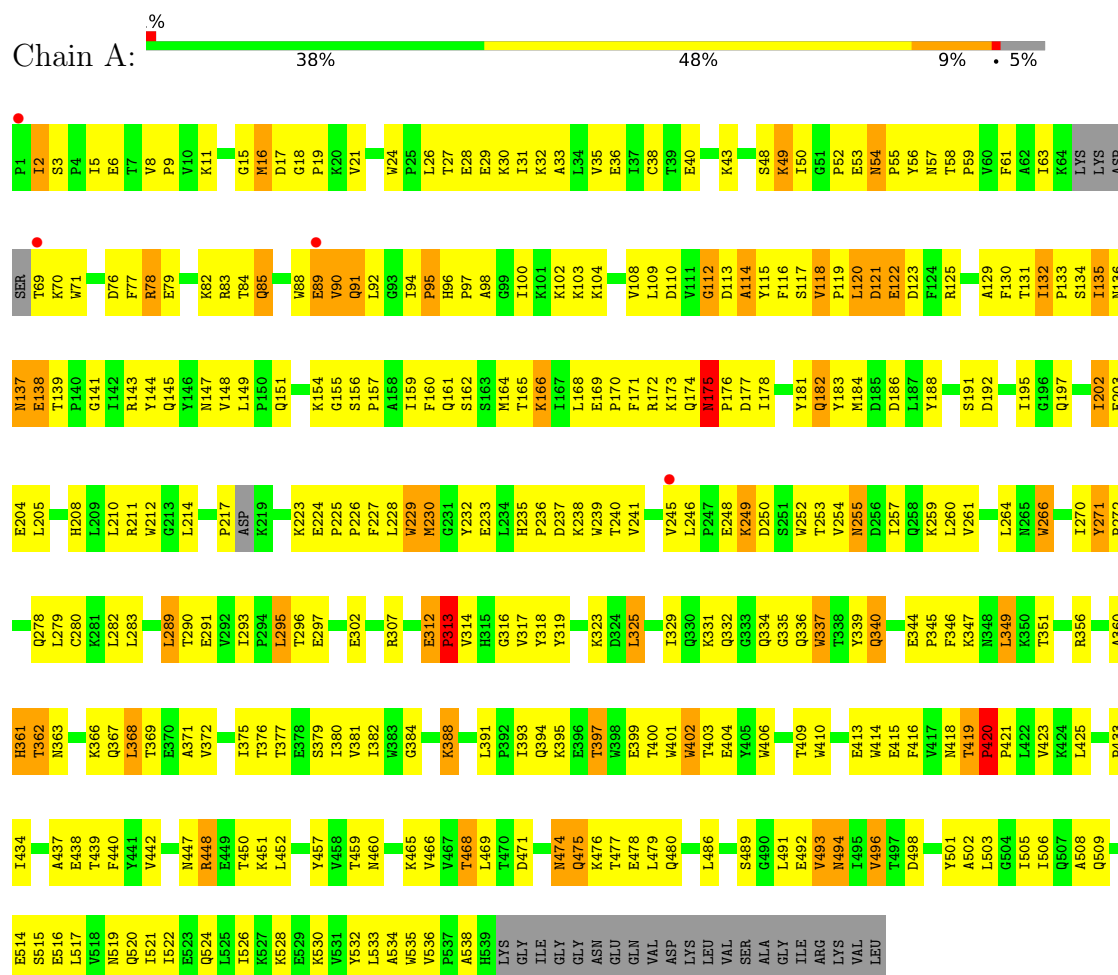
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	28	Total	O	0	0
			28	28		

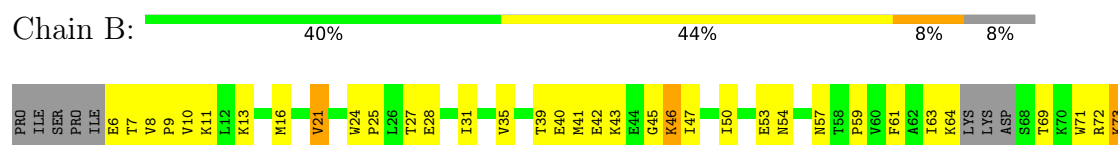
3 Residue-property plots

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: Reverse transcriptase



• Molecule 2: Reverse transcriptase



V365	K366	Q367	L368	T369	E370	A371	V372	E378	V383	G384	K385	T386	P387	F388	F389	K390	L391	P392	T393	Q394	W401	W402	T403	E404	Y405	W406	P412	E413	W414	E415	F416	W417	W418	T419	P420	V423	K424	L425	W426	Y427	Q428	K431	I434	W435	G436	ALA	GLU	THR	PHE								
K281	L282	L283	T286	K287	A288	L289	T296	E297	E298	E302	L303	A304	E305	K306	R307	E308	I309	L310	K311	G316	Y319	D320	P321	K322	K323	D324	L325	I326	A327	E328	Q332	G333	Q336	K337	T338	Y339	Q340	I341	Y342	Q343	L349	K350	K353	G359	K360	K361	D364										
H208	L209	L210	R211	W212	GLY	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	PRO	PHE	LEU	TRP	MET	GLY	TYR	E233	L234	H235	P236	D237	K238	W239	T240	V241	Q242	P243	I244	V245	E248	K249	D250	T253	V254	N255	D256	I257	Q258	W266	A267	Y271	I274	K275	V276	R277	Q278					
Q145	Y146	M147	V148	L149	P150	Q151	G152	W153	P157	L158	D159	F160	W161	S162	S163	P164	T165	K166	I167	L168	E169	G170	F171	R172	K173	Q174	M175	D176	L177	I178	V179	L180	Y181	Q182	Y183	M184	L185	D186	L187	Y188	V189	G190	S191	D192	L193	E194	I195	G196	R199	T200	K201	I202	E203	F204	L205	R206	Q207
L74	V75	D76	F77	R78	E79	K82	R83	T84	Q85	D86	F87	W88	GLU	VAL	GLN	LEU	G93	I94	P97	A98	G99	I100	K101	K104	S105	V106	T107	V108	L109	D110	V111	A114	Y115	F116	S117	V118	P119	L120	D121	E122	R125	K126	T131	I135	N136	N137	F138	T139	P140	R143	Y144						

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.10Å 110.30Å 72.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 2.60 29.51 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (29.51-2.60) 94.0 (29.51-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.57Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.313 0.218 , 0.230	Depositor DCC
R_{free} test set	1632 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7803	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: CSD, TNK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/4477	1.07	30/6085 (0.5%)
2	B	0.54	1/3432 (0.0%)	1.04	19/4661 (0.4%)
All	All	0.54	1/7909 (0.0%)	1.06	49/10746 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	94	ILE	CA-CB	5.72	1.58	1.54

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	417	VAL	N-CA-C	8.66	119.39	108.82
1	A	137	ASN	N-CA-C	-7.89	102.47	113.20
1	A	114	ALA	N-CA-C	-7.83	103.19	112.89
1	A	349	LEU	N-CA-C	-7.72	103.47	113.12
1	A	250	ASP	N-CA-C	-7.62	103.55	112.92
1	A	494	ASN	N-CA-C	-7.52	96.64	108.90
1	A	319	TYR	N-CA-C	7.47	120.84	108.96
1	A	388	LYS	N-CA-C	-7.31	97.32	109.24
2	B	194	GLU	N-CA-C	-7.25	101.49	110.41
2	B	428	GLN	N-CA-C	-7.04	103.61	111.71
2	B	401	TRP	N-CA-C	6.92	121.86	113.41
1	A	132	ILE	CA-C-N	6.82	127.75	120.11
1	A	132	ILE	C-N-CA	6.82	127.75	120.11
2	B	69	THR	N-CA-C	-6.68	105.04	113.72
1	A	131	THR	N-CA-C	6.67	120.50	108.69
1	A	271	TYR	CA-C-N	6.45	127.90	119.84
1	A	271	TYR	C-N-CA	6.45	127.90	119.84
1	A	49	LYS	N-CA-C	-6.38	100.21	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	VAL	N-CA-C	6.34	116.98	108.11
1	A	134	SER	N-CA-C	-6.33	100.83	109.95
1	A	118	VAL	CA-C-N	6.31	126.28	119.78
1	A	118	VAL	C-N-CA	6.31	126.28	119.78
2	B	54	ASN	CA-C-N	6.26	127.17	120.47
2	B	54	ASN	C-N-CA	6.26	127.17	120.47
2	B	186	ASP	N-CA-C	6.15	119.95	110.42
1	A	54	ASN	N-CA-C	-6.04	98.49	108.75
2	B	235	HIS	CA-C-N	6.03	127.38	119.84
2	B	235	HIS	C-N-CA	6.03	127.38	119.84
2	B	297	GLU	N-CA-C	-6.03	104.70	111.28
1	A	118	VAL	N-CA-C	6.00	114.43	107.89
2	B	131	THR	N-CA-C	6.00	119.25	109.06
2	B	250	ASP	N-CA-C	-5.97	104.46	110.97
1	A	175	ASN	CA-C-N	5.70	125.32	119.56
1	A	175	ASN	C-N-CA	5.70	125.32	119.56
2	B	147	ASN	N-CA-C	-5.67	106.90	113.88
2	B	160	PHE	N-CA-C	-5.57	107.07	112.97
1	A	197	GLN	N-CA-C	-5.46	104.36	111.02
1	A	368	LEU	N-CA-C	-5.46	105.23	111.07
1	A	337	TRP	N-CA-C	5.30	117.44	109.23
1	A	297	GLU	N-CA-C	-5.29	105.42	111.14
1	A	382	ILE	N-CA-C	5.22	116.69	111.00
1	A	419	THR	CA-C-N	5.18	125.72	120.38
1	A	419	THR	C-N-CA	5.18	125.72	120.38
2	B	115	TYR	N-CA-C	5.17	117.65	111.71
1	A	204	GLU	N-CA-C	-5.11	105.63	111.14
2	B	316	GLY	N-CA-C	5.08	122.36	115.30
2	B	349	LEU	N-CA-C	-5.04	106.91	113.16
1	A	135	ILE	N-CA-C	5.03	115.75	110.62
2	B	168	LEU	N-CA-C	5.02	119.24	111.56

There are no chirality outliers.

There are no planarity outliers.

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	4370	0	4413	284	1
2	B	3339	0	3367	220	0
3	A	27	0	24	5	0
4	A	39	0	0	2	1
4	B	28	0	0	0	0
All	All	7803	0	7804	493	1

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 32.

All (493) 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:182:GLN:HE21	1:A:182:GLN:C	1.68	1.01
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.59	1.01
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.44	0.98
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.44	0.96
1:A:270:ILE:HG22	1:A:314:VAL:HG21	1.48	0.96
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.46	0.94
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.54	0.90
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.53	0.90
1:A:502:ALA:HA	1:A:505:ILE:HD12	1.55	0.88
2:B:235:HIS:O	2:B:238:LYS:HG2	1.73	0.88
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.13	0.87
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.53	0.87
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.57	0.86
2:B:332:GLN:NE2	2:B:424:LYS:HE2	1.89	0.86
2:B:241:VAL:HG22	2:B:350:LYS:HA	1.57	0.85
1:A:108:VAL:HG11	1:A:223:LYS:HD2	1.59	0.83
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.44	0.83
2:B:366:LYS:O	2:B:370:GLU:HG3	1.79	0.83
1:A:17:ASP:O	1:A:83:ARG:HD3	1.79	0.82
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.61	0.82
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.63	0.81
2:B:31:ILE:O	2:B:35:VAL:HG23	1.81	0.81
1:A:388:LYS:HD2	1:A:413:GLU:OE2	1.81	0.81
1:A:16:MET:CE	1:A:83:ARG:HG2	2.14	0.78
2:B:266:TRP:CH2	2:B:423:VAL:HG22	2.18	0.78
2:B:350:LYS:HE2	2:B:378:GLU:OE1	1.82	0.78
1:A:228:LEU:HD12	1:A:228:LEU:N	1.98	0.78
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.30	0.78
2:B:332:GLN:HE22	2:B:424:LYS:HE2	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.50	0.77
1:A:16:MET:HE3	4:A:1004:HOH:O	1.83	0.77
1:A:278:GLN:O	1:A:282:LEU:HD13	1.85	0.77
2:B:195:ILE:HG23	2:B:196:GLY:H	1.49	0.76
1:A:98:ALA:HB2	1:A:349:LEU:O	1.87	0.74
2:B:163:SER:O	2:B:167:ILE:HG23	1.86	0.74
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.17	0.74
1:A:136:ASN:C	1:A:138:GLU:H	1.91	0.74
1:A:344:GLU:OE1	1:A:347:LYS:HD2	1.86	0.74
1:A:30:LYS:HE2	1:A:71:TRP:CH2	2.23	0.74
1:A:376:THR:O	1:A:380:ILE:HG12	1.88	0.73
1:A:94:ILE:HG21	1:A:230:MET:CE	2.19	0.73
1:A:120:LEU:HD13	1:A:125:ARG:HG2	1.71	0.73
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.18	0.72
1:A:116:PHE:CE2	1:A:151:GLN:HG2	2.25	0.72
1:A:225:PRO:HA	1:A:226:PRO:C	2.12	0.72
1:A:420:PRO:HA	1:A:421:PRO:C	2.14	0.72
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.20	0.71
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.26	0.71
1:A:94:ILE:HG21	1:A:230:MET:HE1	1.72	0.70
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.55	0.70
1:A:19:PRO:O	1:A:56:TYR:HA	1.90	0.70
2:B:139:THR:HG22	2:B:140:PRO:O	1.90	0.70
1:A:516:GLU:O	1:A:520:GLN:HG3	1.92	0.69
2:B:195:ILE:HG23	2:B:196:GLY:N	2.07	0.69
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.75	0.69
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.28	0.69
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.28	0.69
1:A:362:THR:HG22	1:A:363:ASN:H	1.58	0.68
2:B:424:LYS:HD3	2:B:424:LYS:C	2.18	0.68
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.76	0.68
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.07	0.68
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.06	0.68
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.29	0.67
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.77	0.67
1:A:317:VAL:HG12	1:A:318:TYR:N	2.11	0.66
2:B:323:LYS:HB2	2:B:323:LYS:NZ	2.10	0.66
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.76	0.66
1:A:136:ASN:HB2	1:A:138:GLU:HG3	1.77	0.66
2:B:35:VAL:O	2:B:39:THR:HG23	1.96	0.66
2:B:208:HIS:O	2:B:211:ARG:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.31	0.65
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.60	0.65
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.11	0.65
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.77	0.65
1:A:40:GLU:HA	1:A:43:LYS:HE2	1.79	0.65
1:A:312:GLU:N	1:A:313:PRO:HD3	2.12	0.65
1:A:63:ILE:HA	1:A:71:TRP:HZ3	1.62	0.65
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.32	0.64
2:B:78:ARG:O	2:B:82:LYS:HG3	1.96	0.64
1:A:11:LYS:O	1:A:85:GLN:HB3	1.97	0.64
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.78	0.64
2:B:61:PHE:HE1	2:B:74:LEU:HD23	1.63	0.64
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.64
1:A:271:TYR:OH	1:A:313:PRO:HA	1.98	0.64
1:A:323:LYS:NZ	1:A:344:GLU:HG2	2.13	0.64
2:B:365:VAL:O	2:B:369:THR:HG23	1.98	0.64
1:A:451:LYS:HD3	1:A:471:ASP:OD2	1.98	0.63
2:B:195:ILE:HG12	2:B:199:ARG:HH21	1.62	0.63
1:A:475:GLN:HG3	1:A:476:LYS:N	2.12	0.63
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.33	0.63
1:A:255:ASN:O	1:A:259:LYS:HG2	1.99	0.62
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.46	0.62
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.80	0.62
1:A:79:GLU:HB3	1:A:83:ARG:NH1	2.14	0.62
1:A:257:ILE:O	1:A:261:VAL:HG23	2.00	0.62
1:A:2:ILE:HG22	1:A:3:SER:N	2.14	0.62
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.81	0.62
2:B:97:PRO:C	2:B:99:GLY:H	2.07	0.61
2:B:73:LYS:NZ	2:B:73:LYS:HB3	2.14	0.61
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.14	0.61
1:A:503:LEU:HD13	1:A:535:TRP:CG	2.36	0.61
1:A:28:GLU:O	1:A:32:LYS:HG3	2.01	0.60
2:B:278:GLN:NE2	2:B:281:LYS:HD2	2.15	0.60
2:B:319:TYR:HE1	2:B:321:PRO:HG3	1.66	0.60
1:A:90:VAL:O	1:A:91:GLN:C	2.44	0.60
1:A:368:LEU:O	1:A:372:VAL:HG23	2.01	0.60
2:B:368:LEU:O	2:B:372:VAL:HG23	2.01	0.60
2:B:308:GLU:O	2:B:311:LYS:HB2	2.01	0.60
2:B:434:ILE:HG22	2:B:435:VAL:HG13	1.82	0.60
1:A:536:VAL:HG12	2:B:258:GLN:HB3	1.83	0.60
2:B:79:GLU:O	2:B:83:ARG:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:O	2:B:258:GLN:HG3	2.00	0.60
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.12	0.60
1:A:40:GLU:HA	1:A:43:LYS:CE	2.32	0.60
1:A:228:LEU:N	1:A:228:LEU:CD1	2.64	0.59
2:B:424:LYS:HZ3	2:B:425:LEU:HD12	1.66	0.59
1:A:312:GLU:N	1:A:313:PRO:CD	2.64	0.59
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.14	0.59
1:A:260:LEU:HG	1:A:264:LEU:CD2	2.33	0.59
1:A:419:THR:HG22	1:A:419:THR:O	2.02	0.59
2:B:97:PRO:O	2:B:99:GLY:N	2.36	0.59
2:B:423:VAL:O	2:B:427:TYR:HD2	1.83	0.59
1:A:371:ALA:O	1:A:375:ILE:HG13	2.03	0.59
2:B:94:ILE:HD11	2:B:182:GLN:H	1.68	0.59
2:B:203:GLU:HA	2:B:206:ARG:HB2	1.85	0.59
1:A:246:LEU:O	1:A:307:ARG:NH1	2.32	0.59
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.32	0.58
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.83	0.58
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.34	0.58
1:A:122:GLU:N	1:A:122:GLU:OE1	2.36	0.58
1:A:2:ILE:HG22	1:A:3:SER:H	1.69	0.58
1:A:116:PHE:HE2	1:A:151:GLN:HG2	1.67	0.58
2:B:88:TRP:CZ3	2:B:93:GLY:N	2.71	0.58
1:A:48:SER:O	1:A:144:TYR:HA	2.03	0.58
1:A:418:ASN:C	1:A:420:PRO:HD3	2.29	0.58
2:B:27:THR:O	2:B:31:ILE:HG13	2.03	0.58
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.04	0.58
1:A:33:ALA:O	1:A:36:GLU:HB3	2.04	0.57
2:B:98:ALA:HA	2:B:101:LYS:NZ	2.19	0.57
1:A:522:ILE:O	1:A:526:ILE:HG13	2.04	0.57
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.38	0.57
1:A:182:GLN:C	1:A:182:GLN:NE2	2.51	0.57
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.40	0.57
1:A:323:LYS:HZ3	1:A:344:GLU:HG2	1.69	0.57
2:B:169:GLU:HG2	2:B:173:LYS:HZ3	1.70	0.57
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.85	0.57
1:A:380:ILE:O	1:A:384:GLY:HA2	2.05	0.57
2:B:332:GLN:NE2	2:B:428:GLN:HB2	2.19	0.56
2:B:160:PHE:O	2:B:160:PHE:CD1	2.57	0.56
1:A:162:SER:O	1:A:165:THR:HB	2.06	0.56
1:A:114:ALA:O	1:A:117:SER:HB2	2.05	0.56
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:MET:O	2:B:168:LEU:HG	2.05	0.56
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.40	0.56
2:B:241:VAL:CG2	2:B:350:LYS:HA	2.33	0.56
2:B:173:LYS:O	2:B:176:PRO:HD3	2.06	0.56
1:A:188:TYR:CD2	3:A:999:TNK:H2	2.41	0.56
1:A:122:GLU:H	1:A:122:GLU:CD	2.15	0.55
1:A:492:GLU:HA	1:A:530:LYS:O	2.06	0.55
1:A:254:VAL:HB	1:A:289:LEU:HA	1.87	0.55
2:B:97:PRO:C	2:B:99:GLY:N	2.64	0.55
2:B:202:ILE:O	2:B:205:LEU:N	2.38	0.55
1:A:202:ILE:HG22	1:A:203:GLU:N	2.22	0.55
1:A:110:ASP:O	1:A:217:PRO:HD2	2.06	0.55
1:A:289:LEU:H	1:A:289:LEU:HD22	1.70	0.55
2:B:50:ILE:CG1	2:B:143:ARG:HB3	2.37	0.55
2:B:205:LEU:HD13	2:B:209:LEU:HD22	1.88	0.55
1:A:233:GLU:HB2	1:A:240:THR:OG1	2.06	0.55
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.37	0.55
2:B:107:THR:O	2:B:189:VAL:HG23	2.06	0.55
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.88	0.55
2:B:13:LYS:HE2	2:B:86:ASP:OD2	2.07	0.55
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.42	0.55
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.87	0.55
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.42	0.54
2:B:278:GLN:HE21	2:B:278:GLN:HA	1.70	0.54
2:B:178:ILE:HG23	2:B:190:GLY:O	2.07	0.54
2:B:257:ILE:HB	2:B:283:LEU:HD11	1.89	0.54
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.36	0.54
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.90	0.54
2:B:423:VAL:O	2:B:427:TYR:CD2	2.61	0.54
1:A:108:VAL:CG1	1:A:223:LYS:HD2	2.33	0.53
1:A:112:GLY:C	1:A:114:ALA:H	2.16	0.53
2:B:323:LYS:HB2	2:B:323:LYS:HZ2	1.72	0.53
2:B:97:PRO:O	2:B:100:ILE:HG22	2.09	0.53
1:A:293:ILE:N	1:A:293:ILE:HD12	2.22	0.53
2:B:43:LYS:C	2:B:45:GLY:H	2.17	0.53
2:B:328:GLU:O	2:B:339:TYR:HA	2.08	0.53
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.89	0.53
1:A:248:GLU:O	1:A:249:LYS:HG3	2.08	0.53
1:A:486:LEU:O	1:A:528:LYS:NZ	2.42	0.53
2:B:57:ASN:HD21	2:B:131:THR:CB	2.22	0.53
2:B:111:VAL:HG22	2:B:185:ASP:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLY:O	1:A:114:ALA:N	2.38	0.53
2:B:94:ILE:HD11	2:B:181:TYR:HD2	1.74	0.53
2:B:98:ALA:HA	2:B:101:LYS:HZ3	1.74	0.53
1:A:169:GLU:O	1:A:173:LYS:HG3	2.09	0.53
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.43	0.53
1:A:27:THR:O	1:A:31:ILE:HG13	2.09	0.53
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.90	0.53
2:B:46:LYS:HE2	2:B:116:PHE:HD2	1.74	0.53
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.44	0.53
1:A:331:LYS:CE	1:A:334:GLN:HA	2.38	0.52
1:A:476:LYS:O	1:A:480:GLN:HB2	2.08	0.52
2:B:88:TRP:CE3	2:B:88:TRP:HA	2.44	0.52
2:B:420:PRO:HB2	2:B:423:VAL:CG2	2.33	0.52
1:A:252:TRP:NE1	1:A:295:LEU:HD11	2.25	0.52
2:B:305:GLU:O	2:B:309:ILE:HG13	2.10	0.52
1:A:171:PHE:O	1:A:175:ASN:ND2	2.43	0.52
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.10	0.52
1:A:502:ALA:HA	1:A:505:ILE:CD1	2.33	0.52
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.44	0.52
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.75	0.52
1:A:94:ILE:HG21	1:A:230:MET:HE2	1.92	0.52
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.92	0.52
2:B:10:VAL:HG11	2:B:153:TRP:CZ2	2.44	0.52
1:A:289:LEU:HD22	1:A:289:LEU:N	2.25	0.52
1:A:474:ASN:O	1:A:478:GLU:HG3	2.09	0.52
2:B:271:TYR:HB2	2:B:274:ILE:CD1	2.40	0.52
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.43	0.52
1:A:514:GLU:HG3	1:A:515:SER:N	2.26	0.51
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.45	0.51
1:A:181:TYR:HB3	1:A:188:TYR:HB2	1.91	0.51
2:B:195:ILE:HG12	2:B:199:ARG:NH2	2.24	0.51
1:A:402:TRP:CD1	1:A:402:TRP:C	2.89	0.51
1:A:77:PHE:O	1:A:78:ARG:C	2.54	0.51
1:A:182:GLN:HE21	1:A:183:TYR:N	2.08	0.51
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.46	0.51
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.45	0.51
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.92	0.51
2:B:401:TRP:O	2:B:404:GLU:N	2.37	0.51
2:B:248:GLU:HG2	2:B:307:ARG:CZ	2.40	0.51
2:B:205:LEU:O	2:B:208:HIS:HB3	2.12	0.50
1:A:317:VAL:CG1	1:A:318:TYR:N	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:GLY:HA2	2:B:361:HIS:CE1	2.46	0.50
1:A:49:LYS:HA	1:A:143:ARG:O	2.11	0.50
1:A:253:THR:HB	1:A:290:THR:O	2.11	0.50
2:B:11:LYS:N	2:B:85:GLN:OE1	2.41	0.50
1:A:363:ASN:O	1:A:366:LYS:HB3	2.10	0.50
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.92	0.50
2:B:169:GLU:O	2:B:172:ARG:N	2.44	0.50
1:A:186:ASP:CG	1:A:223:LYS:HE3	2.35	0.50
2:B:205:LEU:CD1	2:B:209:LEU:HD22	2.42	0.50
2:B:413:GLU:HA	2:B:413:GLU:OE2	2.11	0.50
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.47	0.50
2:B:88:TRP:HA	2:B:88:TRP:HE3	1.75	0.50
2:B:125:ARG:NE	2:B:147:ASN:HA	2.27	0.50
2:B:195:ILE:CG2	2:B:196:GLY:H	2.21	0.50
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.94	0.49
1:A:122:GLU:HA	1:A:125:ARG:NE	2.27	0.49
1:A:168:LEU:O	1:A:172:ARG:HG3	2.11	0.49
1:A:266:TRP:CD1	1:A:266:TRP:C	2.90	0.49
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.37	0.49
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.11	0.49
1:A:89:GLU:HG3	1:A:89:GLU:O	2.12	0.49
2:B:131:THR:HG1	2:B:143:ARG:HH11	1.58	0.49
2:B:24:TRP:HB2	2:B:25:PRO:HD2	1.93	0.49
2:B:349:LEU:O	2:B:350:LYS:HB2	2.12	0.49
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.75	0.49
1:A:63:ILE:CA	1:A:71:TRP:HZ3	2.24	0.49
2:B:16:MET:HE3	2:B:83:ARG:HG2	1.95	0.49
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.47	0.49
2:B:53:GLU:CD	2:B:53:GLU:H	2.21	0.49
1:A:155:GLY:O	1:A:159:ILE:HG13	2.13	0.49
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.42	0.49
2:B:169:GLU:O	2:B:173:LYS:HD3	2.13	0.49
2:B:195:ILE:CD1	2:B:199:ARG:NE	2.75	0.49
1:A:79:GLU:O	1:A:82:LYS:HG2	2.12	0.49
1:A:235:HIS:HB2	1:A:238:LYS:O	2.13	0.49
1:A:508:ALA:O	1:A:509:GLN:C	2.56	0.49
1:A:95:PRO:HG3	2:B:136:ASN:O	2.13	0.48
2:B:6:GLU:OE1	2:B:6:GLU:HA	2.12	0.48
1:A:457:TYR:CD1	1:A:457:TYR:C	2.91	0.48
1:A:448:ARG:NE	1:A:474:ASN:HB2	2.28	0.48
2:B:104:LYS:NZ	2:B:192:ASP:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:PHE:HE1	2:B:151:GLN:CD	2.20	0.48
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.43	0.48
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.95	0.48
1:A:317:VAL:CG2	1:A:347:LYS:HB3	2.38	0.48
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.96	0.48
1:A:283:LEU:N	1:A:283:LEU:HD12	2.28	0.48
2:B:109:LEU:HD11	2:B:205:LEU:HD12	1.95	0.48
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.14	0.48
1:A:340:GLN:CB	1:A:351:THR:HG22	2.44	0.48
2:B:10:VAL:HG11	2:B:153:TRP:HZ2	1.79	0.48
1:A:181:TYR:HB2	3:A:999:TNK:H161	1.96	0.48
1:A:332:GLN:O	1:A:332:GLN:HG2	2.14	0.48
1:A:438:GLU:OE1	1:A:459:THR:OG1	2.30	0.48
2:B:169:GLU:CG	2:B:173:LYS:HZ3	2.27	0.48
1:A:26:LEU:O	1:A:31:ILE:HD11	2.13	0.47
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.48	0.47
1:A:360:ALA:O	1:A:361:HIS:HB3	2.14	0.47
2:B:242:GLN:HA	2:B:242:GLN:OE1	2.13	0.47
2:B:325:LEU:HA	2:B:343:GLN:HG2	1.96	0.47
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.96	0.47
1:A:289:LEU:H	1:A:289:LEU:CD2	2.26	0.47
2:B:333:GLY:O	2:B:336:GLN:HB2	2.14	0.47
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.96	0.47
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.78	0.47
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.95	0.47
1:A:57:ASN:HA	1:A:129:ALA:O	2.15	0.47
2:B:94:ILE:HD11	2:B:181:TYR:CD2	2.49	0.47
2:B:125:ARG:HG2	2:B:146:TYR:O	2.15	0.47
1:A:460:ASN:HA	2:B:286:THR:O	2.14	0.47
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.45	0.47
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.44	0.47
2:B:73:LYS:HB3	2:B:73:LYS:HZ3	1.80	0.47
2:B:136:ASN:O	2:B:137:ASN:HB2	2.15	0.47
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.49	0.47
2:B:368:LEU:O	2:B:371:ALA:HB3	2.14	0.47
1:A:79:GLU:HA	1:A:82:LYS:HG2	1.96	0.47
1:A:379:SER:O	1:A:380:ILE:C	2.57	0.47
2:B:241:VAL:HG12	2:B:241:VAL:O	2.15	0.47
2:B:254:VAL:O	2:B:255:ASN:C	2.58	0.47
2:B:332:GLN:HE22	2:B:428:GLN:HB2	1.79	0.47
2:B:401:TRP:O	2:B:402:TRP:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:TYR:CD1	1:A:339:TYR:C	2.93	0.47
2:B:276:VAL:HA	2:B:302:GLU:OE2	2.14	0.46
1:A:50:ILE:HG21	1:A:145:GLN:HG2	1.98	0.46
1:A:58:THR:HG23	1:A:76:ASP:O	2.15	0.46
1:A:447:ASN:O	1:A:451:LYS:N	2.48	0.46
1:A:409:THR:O	1:A:410:TRP:HB2	2.14	0.46
2:B:169:GLU:HA	2:B:173:LYS:HZ2	1.79	0.46
1:A:8:VAL:O	1:A:121:ASP:HB2	2.15	0.46
1:A:312:GLU:H	1:A:313:PRO:HD3	1.81	0.46
2:B:173:LYS:HD2	2:B:173:LYS:N	2.30	0.46
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.29	0.46
1:A:3:SER:HB3	1:A:5:ILE:CG1	2.37	0.46
2:B:116:PHE:HE1	2:B:151:GLN:CG	2.28	0.46
1:A:356:ARG:NH1	1:A:356:ARG:CG	2.78	0.46
1:A:169:GLU:HB2	1:A:170:PRO:HD3	1.97	0.46
2:B:168:LEU:O	2:B:169:GLU:C	2.58	0.46
2:B:173:LYS:C	2:B:175:ASN:N	2.72	0.46
1:A:118:VAL:O	1:A:148:VAL:HB	2.16	0.46
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.97	0.46
1:A:362:THR:HG22	1:A:363:ASN:N	2.28	0.46
1:A:415:GLU:HG2	1:A:416:PHE:O	2.16	0.46
2:B:125:ARG:O	2:B:126:LYS:C	2.59	0.46
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.46	0.45
1:A:317:VAL:HG12	1:A:318:TYR:O	2.17	0.45
1:A:345:PRO:O	1:A:346:PHE:HB2	2.17	0.45
2:B:195:ILE:CG1	2:B:199:ARG:NE	2.78	0.45
2:B:245:VAL:O	2:B:245:VAL:HG23	2.16	0.45
2:B:326:ILE:HG22	2:B:327:ALA:N	2.31	0.45
1:A:257:ILE:HG22	1:A:283:LEU:HD11	1.97	0.45
1:A:468:THR:O	1:A:469:LEU:HD23	2.16	0.45
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.16	0.45
2:B:158:ALA:O	2:B:161:GLN:HB2	2.16	0.45
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.97	0.45
1:A:434:ILE:CG2	1:A:437:ALA:HB2	2.46	0.45
1:A:15:GLY:O	1:A:16:MET:C	2.60	0.45
1:A:136:ASN:C	1:A:138:GLU:N	2.61	0.45
1:A:208:HIS:O	1:A:211:ARG:HB3	2.16	0.45
2:B:39:THR:O	2:B:42:GLU:HB3	2.17	0.45
1:A:58:THR:CG2	1:A:76:ASP:O	2.65	0.45
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.99	0.45
1:A:118:VAL:HB	1:A:149:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:THR:HG23	2:B:140:PRO:CD	2.47	0.45
1:A:100:ILE:HD12	2:B:136:ASN:HD21	1.82	0.44
1:A:418:ASN:O	1:A:420:PRO:HD3	2.17	0.44
1:A:516:GLU:O	1:A:519:ASN:HB2	2.18	0.44
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.87	0.44
1:A:120:LEU:O	1:A:122:GLU:N	2.50	0.44
1:A:317:VAL:HG12	1:A:318:TYR:H	1.78	0.44
1:A:498:ASP:HA	1:A:536:VAL:O	2.17	0.44
2:B:118:VAL:HG12	2:B:119:PRO:O	2.18	0.44
1:A:181:TYR:CZ	1:A:183:TYR:HB2	2.52	0.44
1:A:340:GLN:HA	1:A:351:THR:HA	1.99	0.44
2:B:169:GLU:C	2:B:173:LYS:HD3	2.43	0.44
2:B:239:TRP:CH2	2:B:378:GLU:HA	2.52	0.44
1:A:169:GLU:N	1:A:170:PRO:CD	2.79	0.44
2:B:63:ILE:HG13	2:B:72:ARG:HB3	1.97	0.44
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.86	0.44
2:B:332:GLN:HE22	2:B:424:LYS:CE	2.24	0.44
2:B:105:SER:HA	2:B:234:LEU:O	2.17	0.44
1:A:177:ASP:C	1:A:178:ILE:HD12	2.42	0.44
2:B:303:LEU:HD13	2:B:307:ARG:NH2	2.33	0.44
1:A:115:TYR:CG	1:A:151:GLN:NE2	2.86	0.44
1:A:399:GLU:O	1:A:403:THR:HB	2.17	0.44
2:B:163:SER:O	2:B:167:ILE:CG2	2.62	0.44
1:A:63:ILE:HD12	1:A:63:ILE:O	2.18	0.44
2:B:435:VAL:HG23	2:B:436:GLY:N	2.33	0.44
1:A:100:ILE:HG12	3:A:999:TNK:H6	1.99	0.44
1:A:279:LEU:CD2	1:A:302:GLU:OE1	2.66	0.44
1:A:63:ILE:HD12	1:A:63:ILE:C	2.43	0.43
2:B:46:LYS:CE	2:B:116:PHE:HD2	2.31	0.43
2:B:159:ILE:C	2:B:161:GLN:H	2.26	0.43
1:A:54:ASN:C	1:A:56:TYR:N	2.76	0.43
1:A:161:GLN:HA	1:A:161:GLN:OE1	2.18	0.43
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.53	0.43
2:B:388:LYS:HE2	2:B:415:GLU:HB3	2.00	0.43
1:A:434:ILE:HB	1:A:437:ALA:HB3	2.01	0.43
1:A:228:LEU:HD12	1:A:228:LEU:H	1.81	0.43
1:A:479:LEU:O	1:A:521:ILE:HD11	2.18	0.43
2:B:353:LYS:HE3	2:B:353:LYS:HB2	1.84	0.43
1:A:377:THR:O	1:A:381:VAL:HG23	2.18	0.43
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.84	0.43
2:B:43:LYS:C	2:B:45:GLY:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:ARG:HG2	2:B:278:GLN:H	1.84	0.43
1:A:132:ILE:HA	1:A:133:PRO:HD3	1.84	0.43
1:A:161:GLN:O	1:A:162:SER:C	2.61	0.43
2:B:170:PRO:O	2:B:174:GLN:HG3	2.18	0.43
1:A:112:GLY:C	1:A:114:ALA:N	2.77	0.43
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.64	0.43
2:B:245:VAL:HG13	2:B:431:LYS:HB2	2.01	0.43
1:A:232:TYR:HA	1:A:240:THR:O	2.19	0.43
2:B:108:VAL:HA	2:B:187:LEU:O	2.18	0.43
2:B:404:GLU:HB2	2:B:405:TYR:CE1	2.54	0.43
1:A:228:LEU:CD1	1:A:228:LEU:H	2.31	0.43
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.54	0.43
2:B:320:ASP:OD1	2:B:320:ASP:C	2.61	0.43
1:A:159:ILE:O	1:A:160:PHE:C	2.60	0.42
1:A:229:TRP:O	1:A:232:TYR:HB2	2.18	0.42
1:A:254:VAL:HB	1:A:289:LEU:O	2.18	0.42
1:A:400:THR:O	1:A:403:THR:HG22	2.19	0.42
1:A:439:THR:HA	1:A:494:ASN:HB2	2.01	0.42
1:A:465:LYS:HG2	1:A:466:VAL:N	2.33	0.42
1:A:182:GLN:NE2	1:A:183:TYR:N	2.67	0.42
1:A:317:VAL:CG1	1:A:318:TYR:H	2.33	0.42
2:B:169:GLU:O	2:B:172:ARG:HB2	2.19	0.42
1:A:84:THR:HB	1:A:154:LYS:HD3	2.01	0.42
2:B:8:VAL:HG23	2:B:9:PRO:HD2	2.01	0.42
2:B:406:TRP:CH2	2:B:412:PRO:HD2	2.55	0.42
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.54	0.42
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.74	0.42
1:A:176:PRO:C	1:A:178:ILE:H	2.26	0.42
1:A:24:TRP:CB	1:A:61:PHE:HE1	2.32	0.42
1:A:54:ASN:O	1:A:56:TYR:N	2.52	0.42
1:A:170:PRO:O	1:A:174:GLN:HG3	2.20	0.42
1:A:307:ARG:NH1	1:A:307:ARG:HG2	2.35	0.42
1:A:442:VAL:HG22	1:A:496:VAL:O	2.19	0.42
2:B:253:THR:O	2:B:256:ASP:HB2	2.18	0.42
1:A:236:PRO:HB3	3:A:999:TNK:C22	2.50	0.42
2:B:326:ILE:O	2:B:341:ILE:HA	2.20	0.42
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.85	0.42
1:A:438:GLU:OE1	1:A:459:THR:CB	2.68	0.42
1:A:451:LYS:O	1:A:471:ASP:N	2.53	0.42
2:B:41:MET:HE2	2:B:47:ILE:HG23	2.01	0.42
2:B:278:GLN:HG3	2:B:298:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:SER:HB2	1:A:493:VAL:HG13	2.02	0.42
2:B:139:THR:CG2	2:B:140:PRO:N	2.83	0.42
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.50	0.42
1:A:270:ILE:CG2	1:A:314:VAL:CG2	2.93	0.42
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.53	0.42
3:A:999:TNK:H131	3:A:999:TNK:H172	1.80	0.42
2:B:393:ILE:HG12	2:B:394:GLN:N	2.34	0.42
1:A:9:PRO:HG2	2:B:53:GLU:HG3	2.02	0.41
1:A:28:GLU:HG3	1:A:29:GLU:N	2.35	0.41
1:A:79:GLU:HA	1:A:82:LYS:CD	2.49	0.41
1:A:165:THR:O	1:A:166:LYS:C	2.61	0.41
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.83	0.41
2:B:88:TRP:CH2	2:B:93:GLY:N	2.88	0.41
2:B:389:PHE:HB3	2:B:391:LEU:HD21	2.02	0.41
1:A:94:ILE:HG22	1:A:229:TRP:CH2	2.55	0.41
1:A:137:ASN:O	1:A:137:ASN:CG	2.63	0.41
1:A:393:ILE:HB	1:A:423:VAL:HG22	2.00	0.41
1:A:54:ASN:C	1:A:56:TYR:H	2.27	0.41
1:A:82:LYS:HA	4:A:1007:HOH:O	2.19	0.41
2:B:234:LEU:C	2:B:236:PRO:HD3	2.46	0.41
1:A:70:LYS:HB3	1:A:70:LYS:HE2	1.88	0.41
1:A:254:VAL:HG23	1:A:293:ILE:HD11	2.01	0.41
1:A:496:VAL:HA	1:A:534:ALA:O	2.20	0.41
2:B:369:THR:O	2:B:370:GLU:C	2.64	0.41
1:A:271:TYR:HH	1:A:313:PRO:HA	1.86	0.41
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.20	0.41
1:A:95:PRO:HD2	1:A:229:TRP:HH2	1.85	0.41
1:A:210:LEU:C	1:A:212:TRP:N	2.79	0.41
1:A:279:LEU:HD23	1:A:302:GLU:OE1	2.21	0.41
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.56	0.41
1:A:536:VAL:CG1	2:B:258:GLN:HB3	2.49	0.41
2:B:207:GLN:O	2:B:208:HIS:C	2.63	0.41
1:A:120:LEU:CD2	1:A:121:ASP:N	2.83	0.41
1:A:138:GLU:HB3	1:A:139:THR:H	1.51	0.41
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.21	0.41
1:A:337:TRP:CZ3	1:A:368:LEU:HD23	2.55	0.41
1:A:503:LEU:HD13	1:A:535:TRP:CB	2.50	0.41
2:B:364:ASP:O	2:B:367:GLN:N	2.54	0.41
2:B:424:LYS:C	2:B:424:LYS:CD	2.91	0.41
1:A:95:PRO:HB3	2:B:136:ASN:ND2	2.37	0.40
1:A:181:TYR:CD2	1:A:181:TYR:C	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:O	1:A:261:VAL:C	2.64	0.40
1:A:132:ILE:O	1:A:141:GLY:HA3	2.21	0.40
1:A:253:THR:HA	1:A:291:GLU:O	2.22	0.40
1:A:114:ALA:HA	1:A:117:SER:HB2	2.02	0.40
2:B:169:GLU:O	2:B:170:PRO:C	2.65	0.40
1:A:103:LYS:HB3	1:A:191:SER:O	2.21	0.40
1:A:401:TRP:HB2	1:A:425:LEU:HD21	2.03	0.40
2:B:166:LYS:C	2:B:168:LEU:N	2.79	0.40
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.57	0.40
1:A:96:HIS:CD2	1:A:98:ALA:H	2.40	0.40
1:A:486:LEU:HB3	1:A:524:GLN:HB3	2.03	0.40
2:B:46:LYS:HG2	2:B:116:PHE:CD2	2.56	0.40
2:B:151:GLN:H	2:B:151:GLN:HG3	1.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:OE1	4:A:1057:HOH:O[1_556]	2.15	0.05

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	527/560 (94%)	460 (87%)	49 (9%)	18 (3%)	3	4
2	B	396/440 (90%)	344 (87%)	45 (11%)	7 (2%)	6	14
All	All	923/1000 (92%)	804 (87%)	94 (10%)	25 (3%)	4	7

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	138	GLU
1	A	272	PRO
1	A	16	MET
1	A	85	GLN
1	A	112	GLY
1	A	296	THR
1	A	313	PRO
2	B	98	ALA
2	B	361	HIS
1	A	95	PRO
1	A	113	ASP
1	A	361	HIS
1	A	420	PRO
2	B	193	LEU
1	A	78	ARG
1	A	121	ASP
2	B	40	GLU
2	B	166	LYS
2	B	350	LYS
1	A	91	GLN
1	A	52	PRO
1	A	312	GLU
2	B	169	GLU
1	A	55	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	478/499 (96%)	429 (90%)	49 (10%)	7	15
2	B	367/400 (92%)	341 (93%)	26 (7%)	13	31
All	All	845/899 (94%)	770 (91%)	75 (9%)	9	20

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

Mol	Chain	Res	Type
1	A	6	GLU
1	A	53	GLU
1	A	69	THR
1	A	89	GLU
1	A	90	VAL
1	A	92	LEU
1	A	97	PRO
1	A	102	LYS
1	A	109	LEU
1	A	120	LEU
1	A	122	GLU
1	A	123	ASP
1	A	135	ILE
1	A	166	LYS
1	A	175	ASN
1	A	182	GLN
1	A	184	MET
1	A	195	ILE
1	A	202	ILE
1	A	205	LEU
1	A	229	TRP
1	A	230	MET
1	A	237	ASP
1	A	249	LYS
1	A	255	ASN
1	A	266	TRP
1	A	289	LEU
1	A	295	LEU
1	A	313	PRO
1	A	325	LEU
1	A	336	GLN
1	A	340	GLN
1	A	362	THR
1	A	369	THR
1	A	397	THR
1	A	402	TRP
1	A	404	GLU
1	A	420	PRO
1	A	448	ARG
1	A	452	LEU
1	A	468	THR
1	A	474	ASN
1	A	475	GLN

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Mol	Chain	Res	Type
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	501	TYR
1	A	517	LEU
1	A	533	LEU
2	B	21	VAL
2	B	46	LYS
2	B	73	LYS
2	B	82	LYS
2	B	165	THR
2	B	167	ILE
2	B	170	PRO
2	B	187	LEU
2	B	189	VAL
2	B	192	ASP
2	B	194	GLU
2	B	209	LEU
2	B	233	GLU
2	B	234	LEU
2	B	243	PRO
2	B	277	ARG
2	B	283	LEU
2	B	287	LYS
2	B	289	LEU
2	B	303	LEU
2	B	323	LYS
2	B	361	HIS
2	B	368	LEU
2	B	388	LYS
2	B	403	THR
2	B	425	LEU

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

Mol	Chain	Res	Type
1	A	91	GLN
1	A	96	HIS
1	A	136	ASN
1	A	151	GLN
1	A	174	GLN
1	A	175	ASN

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Mol	Chain	Res	Type
1	A	182	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	474	ASN
1	A	475	GLN
1	A	500	GLN
1	A	507	GLN
2	B	57	ASN
2	B	147	ASN
2	B	175	ASN
2	B	197	GLN
2	B	235	HIS
2	B	255	ASN
2	B	258	GLN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	361	HIS
2	B	394	GLN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	A	280	1	4,7,8	1.22	0	1,8,10	4.13	1 (100%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	280	CSD	OD1-SG-CB	4.13	113.21	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

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	TNK	A	999	-	29,29,29	1.91	9 (31%)	32,39,39	0.96	2 (6%)

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	TNK	A	999	-	-	3/14/14/14	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	TNK	C7-C12	5.53	1.41	1.35
3	A	999	TNK	C13-C7	3.23	1.54	1.50
3	A	999	TNK	C17-N8	2.80	1.51	1.46
3	A	999	TNK	C3-C2	2.59	1.43	1.38
3	A	999	TNK	C14-C12	2.52	1.55	1.52
3	A	999	TNK	C4-C3	2.22	1.43	1.38
3	A	999	TNK	C23-C22	2.18	1.43	1.38
3	A	999	TNK	C5-C4	2.18	1.43	1.38
3	A	999	TNK	C9-N8	2.17	1.42	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	TNK	C1-C13-C7	2.61	120.02	114.78
3	A	999	TNK	C14-C12-C7	2.23	126.08	120.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

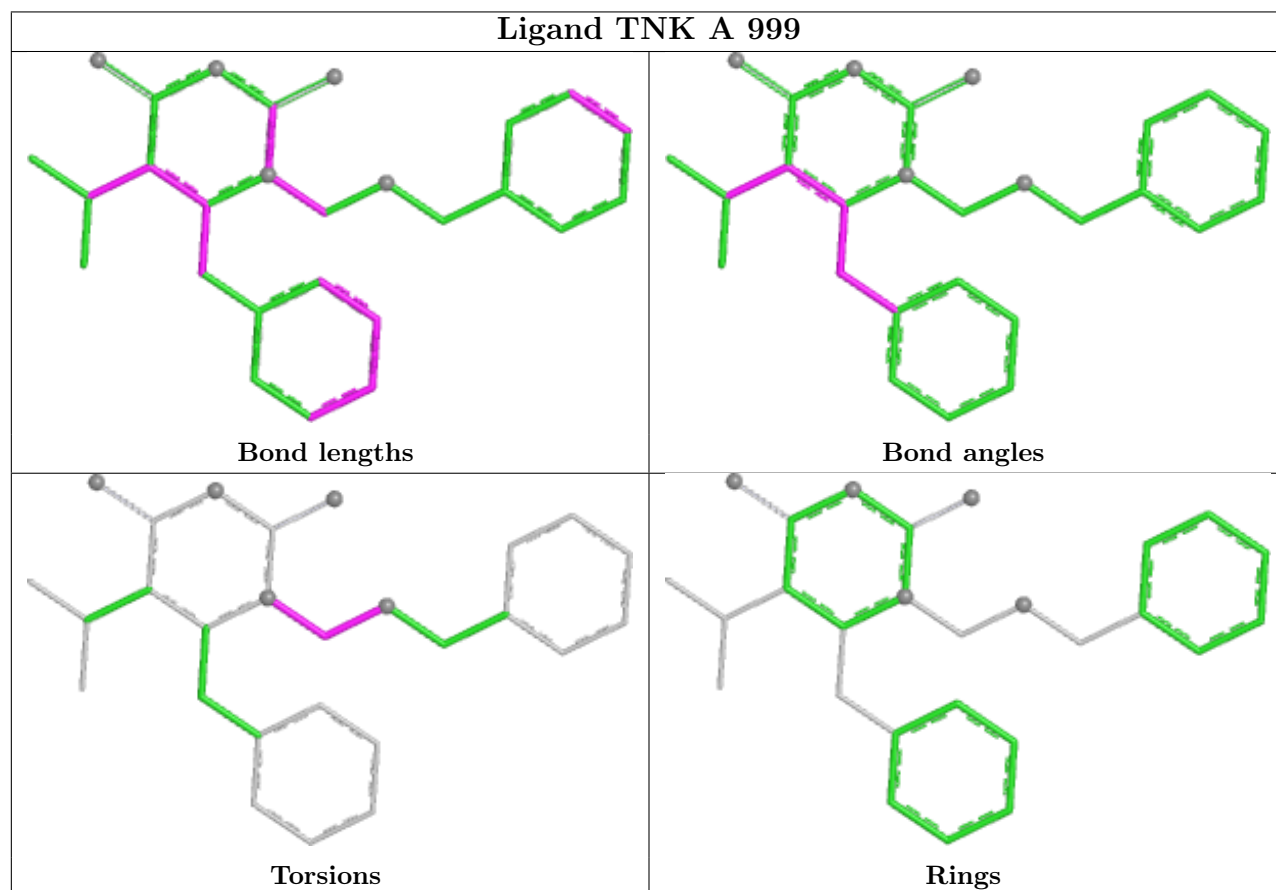
Mol	Chain	Res	Type	Atoms
3	A	999	TNK	O17-C17-N8-C7
3	A	999	TNK	O17-C17-N8-C9
3	A	999	TNK	N8-C17-O17-C18

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	TNK	5	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	533/560 (95%)	-0.21	4 (0%) 82 80	39, 75, 120, 150	0
2	B	404/440 (91%)	-0.26	2 (0%) 87 85	38, 74, 125, 150	0
All	All	937/1000 (93%)	-0.23	6 (0%) 85 83	38, 74, 122, 150	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	93	GLY	2.5
1	A	69	THR	2.3
1	A	1	PRO	2.3
1	A	245	VAL	2.1
1	A	89	GLU	2.0
2	B	88	TRP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.95	0.08	74,75,88,95	0

6.3 Carbohydrates [i](#)

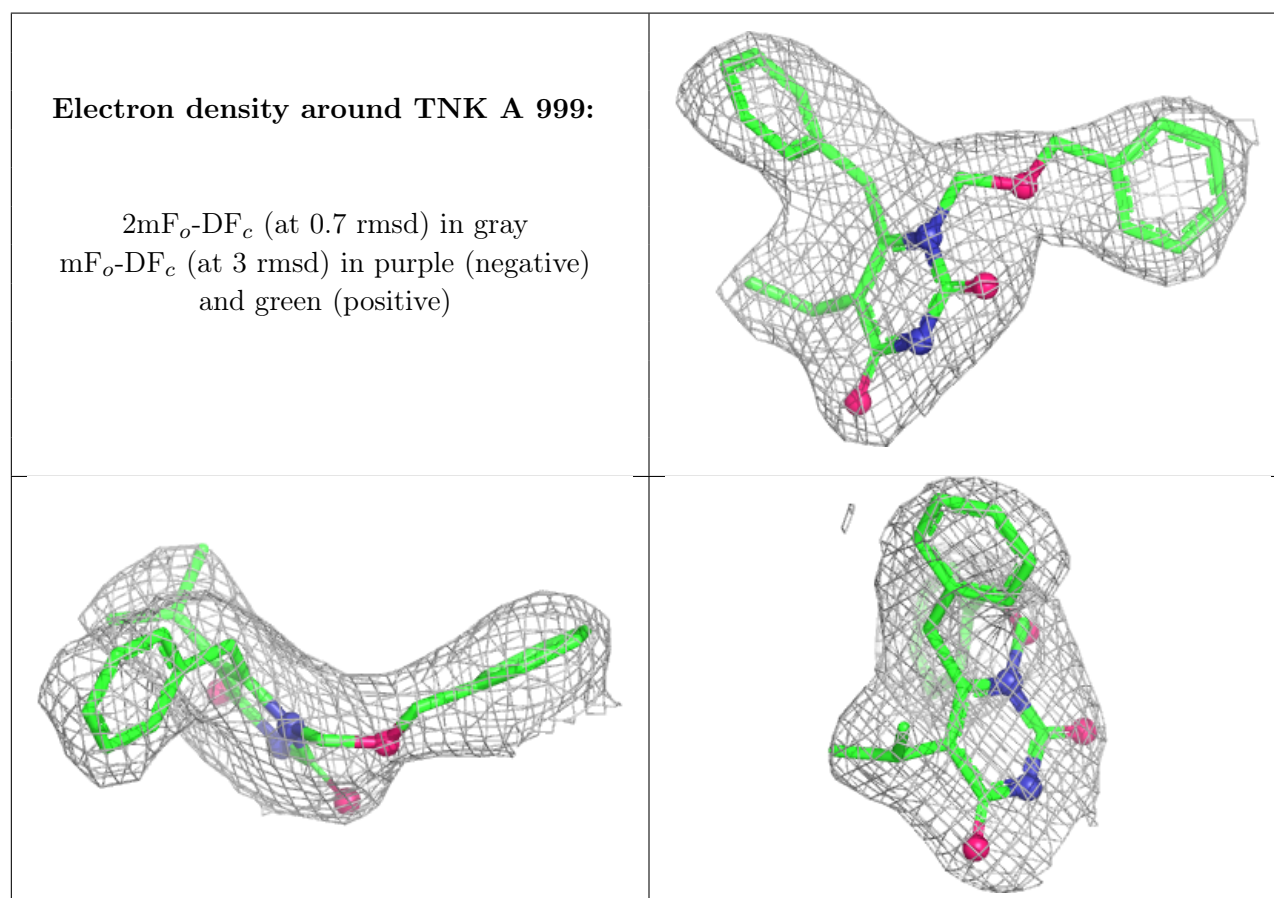
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	TNK	A	999	27/27	0.95	0.08	42,61,82,86	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.