



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:25 AM UTC

PDB ID : 1UWB / pdb_00001uwb
Title : TYR 181 CYS HIV-1 RT/8-CL TIBO
Authors : Das, K.; Ding, J.; Hsiou, Y.; Arnold, E.
Deposited on : 1996-11-21
Resolution : 3.20 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

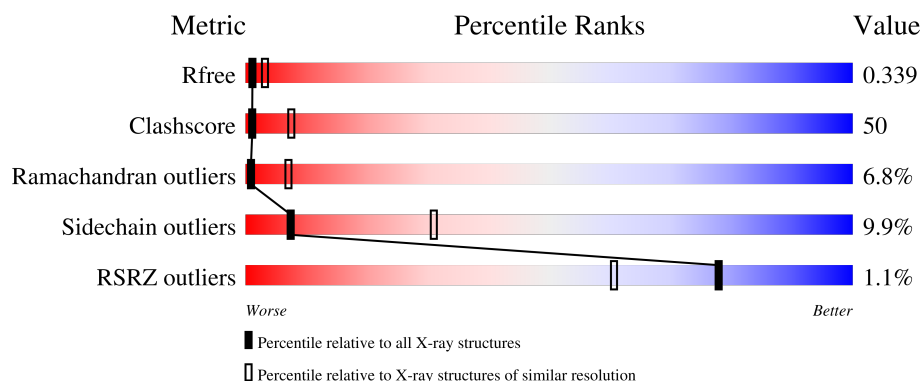
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	558	33% 55% 11% .
2	B	427	24% 56% 18% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7822 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	558	Total	C	N	O	S	0	0	0
			4365	2822	725	812	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	CYS	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

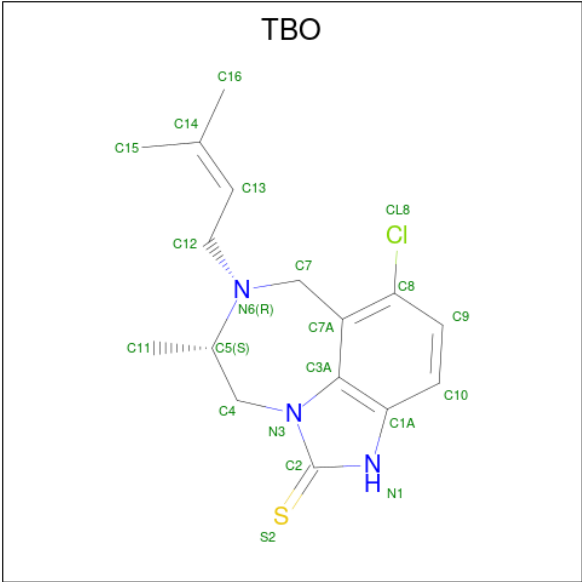
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3436	2234	567	629	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	181	CYS	TYR	engineered mutation	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 5-CHLORO-8-METHYL-7-(3-METHYL-BUT-2-ENYL)-6,7,8,9-TETRAHYDRO-2H-2,7,9A-TRIAZA-BENZO[CD]AZULENE-1-THIONE (CCD ID: TBO) (formula: C₁₆H₂₀ClN₃S).

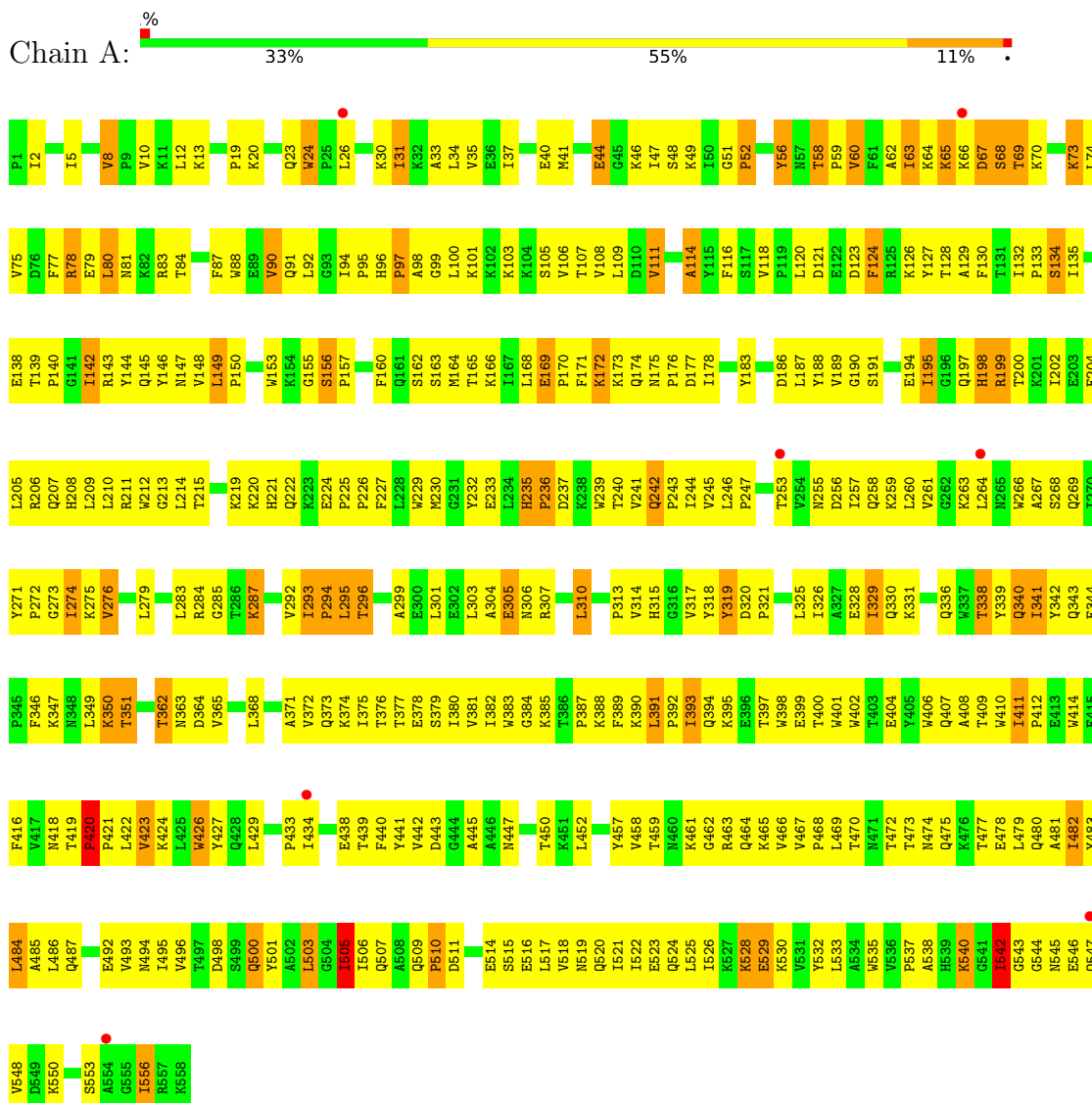


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	S		
3	A	1	21	16	1	3	1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: REVERSE TRANSCRIPTASE



• Molecule 2: REVERSE TRANSCRIPTASE



F389	K390	L391	P392	I393	Q394	K395	E396	T397	W398	E399	T400	W401	W402	T403	E404	W405	W406	Q407	W410	I411	P412	E413	W414	E415	F416	W417	N418	T419	P420	P421	L422	K423	K424	L425	W426	Y427																					
I326	A327	E328	I329	Q330	K331	Q332	Q333	Q336	W337	T338	T339	Q340	I341	Y342	Q343	E344	P345	F346	K347	N348	L349	K350	T351	G352	K353	Y354	A355	R356	K357	T358	G359	N363	D364	V365	K366	Q367	L368	T369	E370	A371	V372	Q373	K374	I375	T376	T377	E378	S379	I380	I381	T382	W383	G384	K385	T386	P387	K388
G262	K263	L264	N265	W266	A267	S268	Q269	L270	Y271	P272	G273	L274	L279	S280	K281	L282	L283	R284	G285	T286	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	V314	H315	G316	V317	Y318	Y319	D320	P321	S322	K323	D324	L325
H198	R199	T200	K201	I202	E203	E204	L205	R206	L207	Q207	H208	L209	L210	W211	G212	G213	L214	T215	T216	P217	K220	K223	E224	P225	P226	F227	L228	W229	W230	G231	Y232	E233	L234	H235	P236	D237	K238	W239	T240	V241	Q242	P243	L244	W245	L246	D250	S251	W252	T253	W254	N255	D256	T257	Q258	K259	L260	V261
I135	N136	M137	E138	T139	P140	G141	I142	R143	Y144	Q145	Y146	N147	V148	L149	G152	Q85	D86	F87	W88	E89	Y90	Q91	L92	G93	I94	P95	H96	P97	A98	G99	L100	K101	K102	K103	P104	T107	V108	L109	D110	V111	Y115	F116	S117	V118	E122	D123	F124	R125	K126	Y127	T128	A129	F130	T131	I132	P133	S134
P1	I2	S3	P4	I5	E6	V10	K11	L12	K13	K20	V21	K22	Q23	L26	T27	E28	E29	K30	I31	K32	A33	L34	V35	E36	I37	C38	T39	E40	M41	E42	K43	E44	G45	K46	I47	S48	K49	I50	G51	P52	E53	N54	P55	Y56	N57	T58	P59	V60	F61	A62	I63	K64	K65	S68	T69		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.70Å 69.20Å 104.90Å 90.00° 106.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20 108.15 – 3.20	Depositor EDS
% Data completeness (in resolution range)	85.0 ((Not available)-3.20) 84.1 (108.15-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.19Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.274 , 0.360 0.260 , 0.339	Depositor DCC
R_{free} test set	1059 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 21.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7822	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: TBO

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	0.69	0/4479	1.22	46/6108 (0.8%)
2	B	0.75	0/3534	1.34	55/4812 (1.1%)
All	All	0.71	0/8013	1.27	101/10920 (0.9%)

There are no bond length outliers.

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	132	ILE	CA-C-N	12.01	132.13	119.76
2	B	132	ILE	C-N-CA	12.01	132.13	119.76
2	B	332	GLN	N-CA-C	11.17	125.02	111.40
2	B	422	LEU	N-CA-C	-11.03	99.03	111.82
2	B	418	ASN	N-CA-C	-10.13	101.18	112.72
2	B	51	GLY	CA-C-N	9.33	128.97	119.82
2	B	51	GLY	C-N-CA	9.33	128.97	119.82
2	B	212	TRP	N-CA-C	9.10	123.98	113.15
1	A	177	ASP	N-CA-C	9.01	122.52	112.97
2	B	343	GLN	N-CA-C	-8.92	102.53	113.41
1	A	198	HIS	N-CA-C	-8.90	101.66	111.36
1	A	287	LYS	N-CA-C	8.87	129.68	110.80
2	B	329	ILE	N-CA-C	8.78	121.27	108.53
1	A	500	GLN	N-CA-C	-8.75	101.69	111.14
1	A	528	LYS	N-CA-C	8.65	120.92	110.19
1	A	175	ASN	CA-C-N	8.54	128.68	119.28
1	A	175	ASN	C-N-CA	8.54	128.68	119.28
2	B	235	HIS	CA-C-N	8.53	128.18	119.82
2	B	235	HIS	C-N-CA	8.53	128.18	119.82
2	B	42	GLU	N-CA-C	-8.19	102.43	111.36
1	A	44	GLU	N-CA-C	-7.92	103.34	113.16
1	A	542	ILE	N-CA-C	-7.62	98.85	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	35	VAL	N-CA-C	-7.51	103.21	110.42
2	B	94	ILE	CA-C-N	7.41	127.34	119.85
2	B	94	ILE	C-N-CA	7.41	127.34	119.85
2	B	197	GLN	N-CA-C	-7.33	102.98	110.97
1	A	220	LYS	N-CA-C	-7.24	101.75	110.44
2	B	58	THR	CA-C-N	7.17	127.20	119.89
2	B	58	THR	C-N-CA	7.17	127.20	119.89
1	A	215	THR	N-CA-C	7.10	119.37	109.15
2	B	344	GLU	CA-C-N	7.08	128.69	119.84
2	B	344	GLU	C-N-CA	7.08	128.69	119.84
2	B	225	PRO	N-CA-CB	7.03	109.89	103.08
1	A	293	ILE	N-CA-C	7.00	114.48	107.55
2	B	295	LEU	N-CA-C	6.82	125.33	110.80
1	A	149	LEU	CA-C-N	6.78	126.76	119.78
1	A	149	LEU	C-N-CA	6.78	126.76	119.78
1	A	293	ILE	CA-C-N	6.70	128.21	119.84
1	A	293	ILE	C-N-CA	6.70	128.21	119.84
1	A	391	LEU	N-CA-C	6.68	120.31	109.15
2	B	175	ASN	CA-C-N	6.65	128.16	119.84
2	B	175	ASN	C-N-CA	6.65	128.16	119.84
1	A	420	PRO	N-CA-C	6.63	118.79	110.70
1	A	24	TRP	N-CA-C	-6.62	96.30	109.60
1	A	118	VAL	CA-C-N	6.59	127.58	120.13
1	A	118	VAL	C-N-CA	6.59	127.58	120.13
1	A	58	THR	CA-C-N	6.57	126.80	119.90
1	A	58	THR	C-N-CA	6.57	126.80	119.90
1	A	147	ASN	N-CA-C	-6.57	103.76	113.61
2	B	192	ASP	N-CA-C	-6.54	104.61	112.59
2	B	226	PRO	N-CA-CB	6.38	109.95	103.25
2	B	96	HIS	CA-C-N	6.37	129.07	120.79
2	B	96	HIS	C-N-CA	6.37	129.07	120.79
1	A	305	GLU	N-CA-C	-6.35	104.28	111.07
1	A	118	VAL	N-CA-C	6.14	114.97	108.95
2	B	301	LEU	N-CA-C	-6.11	104.68	111.71
2	B	287	LYS	N-CA-C	6.08	118.74	110.35
2	B	223	LYS	N-CA-C	-6.07	105.86	113.20
2	B	79	GLU	N-CA-C	6.04	117.55	110.97
2	B	237	ASP	N-CA-C	-5.99	106.06	113.19
1	A	346	PHE	N-CA-C	5.98	119.68	111.54
1	A	235	HIS	CA-C-N	5.95	127.28	119.84
1	A	235	HIS	C-N-CA	5.95	127.28	119.84
1	A	222	GLN	N-CA-C	5.93	117.69	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	133	PRO	N-CA-C	5.77	120.14	111.14
1	A	493	VAL	N-CA-C	5.76	116.66	108.42
1	A	20	LYS	N-CA-C	-5.72	106.20	112.72
2	B	13	LYS	CA-C-N	5.68	126.94	119.84
2	B	13	LYS	C-N-CA	5.68	126.94	119.84
2	B	244	ILE	N-CA-C	-5.62	97.66	109.34
1	A	350	LYS	N-CA-C	5.58	117.58	108.76
1	A	388	LYS	N-CA-C	-5.56	102.06	110.28
2	B	215	THR	N-CA-C	-5.53	98.94	108.56
2	B	87	PHE	N-CA-C	-5.49	106.43	113.01
1	A	65	LYS	N-CA-C	5.48	122.47	110.80
2	B	95	PRO	N-CA-C	5.48	120.09	111.38
1	A	484	LEU	N-CA-C	-5.46	105.01	110.97
1	A	56	TYR	N-CA-C	5.41	118.65	110.64
2	B	401	TRP	N-CA-C	5.40	122.31	110.80
2	B	347	LYS	N-CA-C	-5.37	103.88	110.65
2	B	28	GLU	N-CA-C	-5.36	105.34	111.07
2	B	220	LYS	N-CA-C	5.35	118.03	111.82
2	B	10	VAL	N-CA-C	5.33	116.90	109.55
1	A	409	THR	N-CA-C	5.32	115.16	108.45
2	B	292	VAL	N-CA-C	5.30	115.98	107.98
2	B	65	LYS	N-CA-C	5.30	117.70	110.55
2	B	2	ILE	N-CA-C	5.28	120.31	109.34
1	A	67	ASP	N-CA-C	5.22	121.93	110.80
2	B	375	ILE	N-CA-C	-5.22	105.75	110.82
2	B	53	GLU	N-CA-C	-5.21	106.76	113.01
2	B	320	ASP	CA-C-N	5.19	124.90	119.82
2	B	320	ASP	C-N-CA	5.19	124.90	119.82
1	A	68	SER	N-CA-C	5.18	116.78	110.41
1	A	8	VAL	CA-C-N	5.16	125.96	120.13
1	A	8	VAL	C-N-CA	5.16	125.96	120.13
1	A	319	TYR	N-CA-C	5.13	118.58	109.96
2	B	158	ALA	N-CA-C	-5.13	104.76	111.02
2	B	250	ASP	N-CA-C	-5.12	105.69	111.28
1	A	313	PRO	N-CA-C	5.11	118.59	110.21
1	A	329	ILE	N-CA-C	5.05	117.29	108.95
1	A	503	LEU	N-CA-C	-5.05	104.86	111.02

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	4365	0	4260	410	0
2	B	3436	0	3401	382	0
3	A	21	0	20	8	0
All	All	7822	0	7681	768	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 50.

All (768) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HA	1:A:75:VAL:HG22	1.39	1.03
2:B:180:ILE:HG23	2:B:189:VAL:HG22	1.41	1.00
1:A:272:PRO:HA	1:A:351:THR:HG21	1.43	0.99
1:A:318:TYR:CE2	3:A:559:TBO:H10	2.03	0.93
2:B:12:LEU:HA	2:B:84:THR:HG22	1.48	0.92
1:A:543:GLY:H	2:B:284:ARG:HA	1.33	0.91
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.51	0.91
2:B:340:GLN:HB3	2:B:351:THR:HG22	1.54	0.90
1:A:373:GLN:NE2	2:B:397:THR:HA	1.87	0.90
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.51	0.89
1:A:241:VAL:HG11	1:A:266:TRP:HE1	1.37	0.89
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.53	0.89
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.55	0.88
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.09	0.88
2:B:263:LYS:HE2	2:B:425:LEU:HD13	1.58	0.86
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.11	0.85
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.59	0.85
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.42	0.84
1:A:543:GLY:HA2	1:A:546:GLU:HB3	1.61	0.83
1:A:63:ILE:HG22	1:A:64:LYS:H	1.43	0.82
1:A:399:GLU:HA	1:A:402:TRP:NE1	1.94	0.81
1:A:51:GLY:H	1:A:52:PRO:HD2	1.43	0.81
1:A:253:THR:HA	1:A:292:VAL:HA	1.63	0.81
2:B:258:GLN:HG2	2:B:283:LEU:HD13	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.63	0.81
2:B:344:GLU:HB2	2:B:347:LYS:HB2	1.62	0.80
1:A:341:ILE:HD13	1:A:350:LYS:HB3	1.62	0.80
2:B:326:ILE:HD12	2:B:388:LYS:HE2	1.63	0.80
1:A:101:LYS:HD3	1:A:321:PRO:HD3	1.63	0.80
1:A:257:ILE:HD11	1:A:295:LEU:HD11	1.63	0.80
2:B:132:ILE:CG2	2:B:142:ILE:HB	2.11	0.80
2:B:132:ILE:HG23	2:B:142:ILE:HB	1.62	0.80
2:B:306:ASN:HA	2:B:309:ILE:HB	1.64	0.79
2:B:328:GLU:O	2:B:339:TYR:HA	1.81	0.79
2:B:79:GLU:O	2:B:83:ARG:HG3	1.82	0.79
1:A:164:MET:SD	1:A:168:LEU:HD21	2.23	0.78
1:A:542:ILE:HG23	1:A:545:ASN:HB2	1.66	0.78
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.84	0.78
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.13	0.78
1:A:240:THR:CG2	1:A:315:HIS:HA	2.13	0.77
1:A:8:VAL:O	1:A:121:ASP:HB2	1.85	0.77
2:B:379:SER:HA	2:B:383:TRP:CZ3	2.20	0.77
1:A:106:VAL:HG12	1:A:107:THR:H	1.50	0.77
1:A:227:PHE:O	1:A:233:GLU:HA	1.86	0.76
1:A:317:VAL:HG23	1:A:349:LEU:HD13	1.66	0.76
2:B:79:GLU:HG3	2:B:83:ARG:HD2	1.66	0.76
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.67	0.76
1:A:267:ALA:HB1	1:A:271:TYR:CD2	2.21	0.75
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.21	0.75
1:A:398:TRP:HE1	1:A:411:ILE:HG12	1.50	0.75
1:A:427:TYR:OH	1:A:509:GLN:HA	1.86	0.74
1:A:47:ILE:HG21	1:A:144:TYR:HB3	1.69	0.74
2:B:425:LEU:HD12	2:B:427:TYR:HB3	1.69	0.74
2:B:319:TYR:O	2:B:321:PRO:HD3	1.87	0.74
1:A:543:GLY:HA3	2:B:284:ARG:O	1.88	0.74
2:B:65:LYS:HD2	2:B:407:GLN:HG2	1.70	0.73
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.70	0.73
1:A:503:LEU:O	1:A:507:GLN:HG3	1.86	0.73
1:A:239:TRP:HB3	1:A:318:TYR:HE1	1.53	0.73
1:A:459:THR:OG1	1:A:463:ARG:HB3	1.88	0.73
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.23	0.73
1:A:503:LEU:HD13	1:A:535:TRP:CB	2.18	0.73
2:B:281:LYS:HA	2:B:284:ARG:HG3	1.71	0.72
2:B:254:VAL:O	2:B:258:GLN:HG3	1.90	0.72
1:A:301:LEU:O	1:A:305:GLU:HB2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:PHE:CE1	2:B:76:ASP:HB2	2.24	0.72
1:A:99:GLY:HA2	1:A:383:TRP:NE1	2.03	0.71
2:B:164:MET:SD	2:B:168:LEU:HD11	2.30	0.71
2:B:366:LYS:O	2:B:369:THR:HG22	1.91	0.71
2:B:257:ILE:O	2:B:261:VAL:HG23	1.90	0.71
1:A:169:GLU:O	1:A:172:LYS:HG3	1.91	0.71
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.73	0.70
1:A:47:ILE:CG2	1:A:144:TYR:HB3	2.21	0.70
1:A:256:ASP:HA	1:A:259:LYS:HE3	1.73	0.70
2:B:116:PHE:HA	2:B:148:VAL:HG21	1.74	0.70
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.26	0.70
1:A:246:LEU:HG	1:A:310:LEU:HD22	1.74	0.70
1:A:443:ASP:CB	1:A:548:VAL:HB	2.21	0.70
2:B:198:HIS:O	2:B:202:ILE:HG12	1.92	0.70
2:B:257:ILE:O	2:B:260:LEU:HB3	1.92	0.69
2:B:252:TRP:O	2:B:292:VAL:HA	1.93	0.69
2:B:260:LEU:O	2:B:264:LEU:HG	1.93	0.69
1:A:474:ASN:O	1:A:478:GLU:HG3	1.92	0.69
2:B:84:THR:HG21	2:B:124:PHE:CZ	2.26	0.69
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.73	0.69
2:B:241:VAL:HG13	2:B:351:THR:OG1	1.93	0.69
1:A:88:TRP:CE2	2:B:143:ARG:HD2	2.27	0.69
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.27	0.69
1:A:478:GLU:O	1:A:481:ALA:HB3	1.92	0.69
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.75	0.69
1:A:267:ALA:HB1	1:A:271:TYR:HD2	1.55	0.69
1:A:514:GLU:CD	1:A:514:GLU:H	2.00	0.69
1:A:239:TRP:O	1:A:240:THR:HG23	1.92	0.69
1:A:92:LEU:HD11	2:B:22:LYS:HE3	1.74	0.68
1:A:443:ASP:HB2	1:A:548:VAL:HB	1.74	0.68
2:B:23:GLN:HG3	2:B:133:PRO:HG3	1.75	0.68
2:B:205:LEU:O	2:B:205:LEU:HD12	1.92	0.68
2:B:261:VAL:HA	2:B:264:LEU:HD12	1.75	0.68
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.76	0.68
1:A:397:THR:HG21	1:A:424:LYS:HA	1.76	0.68
1:A:128:THR:HG21	1:A:150:PRO:HG2	1.75	0.68
1:A:232:TYR:HA	1:A:241:VAL:HG22	1.74	0.68
2:B:201:LYS:O	2:B:204:GLU:HB3	1.93	0.68
2:B:125:ARG:HE	2:B:147:ASN:HA	1.59	0.68
2:B:398:TRP:O	2:B:402:TRP:HD1	1.76	0.68
2:B:166:LYS:O	2:B:170:PRO:HD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ILE:O	1:A:525:LEU:HG	1.94	0.67
2:B:108:VAL:HA	2:B:187:LEU:O	1.94	0.67
1:A:90:VAL:HG23	1:A:91:GLN:H	1.58	0.67
1:A:171:PHE:CE2	1:A:205:LEU:HA	2.30	0.67
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.24	0.67
1:A:326:ILE:O	1:A:341:ILE:HA	1.94	0.67
1:A:188:TYR:CB	3:A:559:TBO:H122	2.25	0.67
2:B:107:THR:HA	2:B:232:TYR:O	1.94	0.67
2:B:199:ARG:O	2:B:202:ILE:HB	1.94	0.67
2:B:323:LYS:HB2	2:B:343:GLN:OE1	1.93	0.67
1:A:398:TRP:CE2	1:A:402:TRP:CD1	2.84	0.66
1:A:198:HIS:O	1:A:202:ILE:HG12	1.96	0.66
1:A:31:ILE:HG21	1:A:134:SER:O	1.96	0.66
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.31	0.66
1:A:399:GLU:HA	1:A:402:TRP:HE1	1.58	0.66
1:A:419:THR:HB	1:A:420:PRO:HD2	1.78	0.66
2:B:84:THR:HG21	2:B:124:PHE:HZ	1.61	0.66
2:B:326:ILE:O	2:B:341:ILE:HA	1.96	0.66
1:A:398:TRP:NE1	1:A:411:ILE:HG12	2.11	0.66
2:B:393:ILE:HG12	2:B:394:GLN:N	2.11	0.66
2:B:40:GLU:O	2:B:43:LYS:HB3	1.96	0.65
1:A:207:GLN:HB3	1:A:211:ARG:HH12	1.59	0.65
1:A:240:THR:HG21	1:A:315:HIS:HA	1.76	0.65
2:B:101:LYS:HD2	2:B:382:ILE:HG23	1.79	0.65
2:B:128:THR:CB	2:B:146:TYR:HB2	2.27	0.65
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.78	0.65
2:B:115:TYR:HD2	2:B:156:SER:HB3	1.61	0.65
1:A:303:LEU:HD21	1:A:307:ARG:HH21	1.60	0.65
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.65
2:B:271:TYR:O	2:B:274:ILE:HG22	1.97	0.65
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.33	0.64
2:B:163:SER:O	2:B:167:ILE:HG12	1.98	0.64
2:B:160:PHE:HE2	2:B:164:MET:HG2	1.63	0.64
2:B:379:SER:HA	2:B:383:TRP:CE3	2.32	0.64
2:B:99:GLY:HA2	2:B:102:LYS:HD2	1.80	0.64
1:A:146:TYR:CE2	1:A:150:PRO:HA	2.33	0.64
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.80	0.63
1:A:260:LEU:O	1:A:264:LEU:HG	1.98	0.63
2:B:380:ILE:O	2:B:384:GLY:N	2.31	0.63
1:A:188:TYR:CG	3:A:559:TBO:H122	2.33	0.63
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:THR:HA	1:A:494:ASN:HB2	1.79	0.63
2:B:257:ILE:HD13	2:B:283:LEU:HB3	1.81	0.63
2:B:329:ILE:HD11	2:B:375:ILE:HD11	1.79	0.63
1:A:241:VAL:HG11	1:A:266:TRP:NE1	2.11	0.63
1:A:468:PRO:C	1:A:469:LEU:HG	2.22	0.63
2:B:378:GLU:O	2:B:381:VAL:HB	1.99	0.63
2:B:320:ASP:CG	2:B:323:LYS:HG2	2.23	0.62
2:B:5:ILE:HG22	2:B:6:GLU:H	1.64	0.62
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.80	0.62
2:B:71:TRP:H	2:B:71:TRP:CD1	2.16	0.62
2:B:77:PHE:HD2	2:B:152:GLY:HA3	1.64	0.62
1:A:101:LYS:HD3	1:A:321:PRO:CD	2.28	0.62
1:A:479:LEU:HA	1:A:482:ILE:HD12	1.81	0.62
1:A:194:GLU:O	1:A:197:GLN:N	2.31	0.62
1:A:331:LYS:O	1:A:421:PRO:HG2	1.99	0.62
1:A:466:VAL:HG12	1:A:467:VAL:N	2.15	0.62
1:A:398:TRP:O	1:A:401:TRP:HB3	1.99	0.62
1:A:445:ALA:O	1:A:477:THR:HG21	1.99	0.62
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.33	0.62
1:A:304:ALA:HA	1:A:307:ARG:HB2	1.81	0.62
2:B:160:PHE:CE2	2:B:164:MET:HG2	2.34	0.62
1:A:341:ILE:O	1:A:349:LEU:HB3	1.99	0.62
1:A:420:PRO:HB2	1:A:421:PRO:HD3	1.82	0.61
1:A:478:GLU:O	1:A:482:ILE:HG13	2.00	0.61
1:A:482:ILE:O	1:A:485:ALA:HB3	2.00	0.61
1:A:500:GLN:OE1	1:A:500:GLN:HA	1.98	0.61
1:A:239:TRP:HB3	1:A:318:TYR:CE1	2.36	0.61
2:B:292:VAL:HG12	2:B:294:PRO:HD3	1.83	0.61
1:A:442:VAL:HG21	1:A:485:ALA:HB2	1.83	0.61
1:A:509:GLN:N	1:A:510:PRO:HD3	2.16	0.61
1:A:372:VAL:HA	1:A:375:ILE:HD12	1.82	0.61
2:B:99:GLY:HA2	2:B:102:LYS:CD	2.31	0.61
2:B:115:TYR:HE2	2:B:157:PRO:N	1.99	0.61
2:B:330:GLN:HB2	2:B:332:GLN:HE22	1.65	0.61
2:B:27:THR:HG23	2:B:30:LYS:H	1.65	0.60
2:B:261:VAL:HG22	2:B:279:LEU:HD23	1.83	0.60
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.36	0.60
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.65	0.60
1:A:368:LEU:O	1:A:371:ALA:HB3	2.02	0.60
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.67	0.60
1:A:90:VAL:HG23	1:A:91:GLN:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:HE21	2:B:397:THR:HA	1.67	0.60
2:B:315:HIS:O	2:B:317:VAL:N	2.35	0.60
2:B:31:ILE:HD13	2:B:133:PRO:O	2.02	0.60
1:A:63:ILE:HG22	1:A:64:LYS:N	2.16	0.60
1:A:317:VAL:HG11	1:A:347:LYS:HE3	1.82	0.60
1:A:441:TYR:O	1:A:548:VAL:HG11	2.02	0.60
2:B:375:ILE:O	2:B:378:GLU:HG2	2.02	0.60
1:A:34:LEU:HD22	1:A:60:VAL:HG12	1.82	0.59
2:B:379:SER:HA	2:B:383:TRP:HZ3	1.65	0.59
2:B:354:TYR:HD2	2:B:371:ALA:HB2	1.68	0.59
2:B:325:LEU:H	2:B:325:LEU:CD2	2.15	0.59
1:A:92:LEU:HD11	2:B:22:LYS:CE	2.32	0.59
1:A:37:ILE:O	1:A:41:MET:HG3	2.02	0.59
1:A:268:SER:O	1:A:351:THR:HB	2.03	0.59
1:A:195:ILE:CG2	1:A:199:ARG:HH12	2.16	0.59
1:A:400:THR:O	1:A:404:GLU:HG3	2.02	0.59
1:A:106:VAL:HG12	1:A:107:THR:N	2.17	0.59
1:A:51:GLY:N	1:A:52:PRO:HD2	2.16	0.59
1:A:492:GLU:HG2	1:A:530:LYS:HD2	1.85	0.59
2:B:239:TRP:HB2	2:B:350:LYS:HE3	1.84	0.59
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.66	0.59
1:A:398:TRP:CE2	1:A:402:TRP:HD1	2.20	0.59
1:A:498:ASP:HB3	1:A:545:ASN:HD21	1.68	0.58
2:B:296:THR:HB	2:B:299:ALA:HB3	1.84	0.58
1:A:95:PRO:HG3	2:B:137:ASN:O	2.03	0.58
1:A:480:GLN:HE22	1:A:483:TYR:HD2	1.51	0.58
1:A:482:ILE:HG23	1:A:495:ILE:HG21	1.85	0.58
1:A:503:LEU:HD22	1:A:535:TRP:CG	2.38	0.58
2:B:94:ILE:HG12	2:B:161:GLN:CD	2.28	0.58
2:B:342:TYR:HB3	2:B:348:ASN:CA	2.34	0.58
1:A:5:ILE:HD11	1:A:166:LYS:HD2	1.85	0.58
2:B:32:LYS:O	2:B:35:VAL:HG22	2.04	0.58
2:B:64:LYS:HB3	2:B:68:SER:HA	1.85	0.58
2:B:127:TYR:C	2:B:129:ALA:H	2.12	0.58
1:A:123:ASP:O	1:A:126:LYS:HE3	2.01	0.58
1:A:40:GLU:O	1:A:44:GLU:HG2	2.04	0.58
1:A:56:TYR:O	1:A:129:ALA:HB3	2.04	0.58
1:A:257:ILE:CD1	1:A:295:LEU:HD11	2.32	0.58
1:A:269:GLN:O	1:A:351:THR:N	2.35	0.58
1:A:163:SER:HA	1:A:166:LYS:HD2	1.85	0.58
2:B:81:ASN:ND2	2:B:154:LYS:HG3	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD11	1:A:383:TRP:HB2	1.85	0.57
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.22	0.57
1:A:97:PRO:HA	1:A:100:LEU:HG	1.87	0.57
1:A:461:LYS:O	1:A:463:ARG:N	2.38	0.57
1:A:108:VAL:HA	1:A:187:LEU:O	2.04	0.57
1:A:543:GLY:N	2:B:284:ARG:HA	2.14	0.57
2:B:41:MET:CB	2:B:47:ILE:HG12	2.34	0.57
2:B:325:LEU:HG	2:B:387:PRO:HB3	1.85	0.57
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.39	0.57
1:A:188:TYR:CD2	3:A:559:TBO:H122	2.40	0.57
2:B:380:ILE:HA	2:B:385:LYS:H	1.68	0.57
1:A:162:SER:O	1:A:166:LYS:HG3	2.04	0.57
1:A:199:ARG:HB2	1:A:199:ARG:NH1	2.20	0.57
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.70	0.56
2:B:342:TYR:CB	2:B:348:ASN:HA	2.33	0.56
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.35	0.56
1:A:329:ILE:HG22	1:A:330:GLN:N	2.20	0.56
1:A:379:SER:CB	1:A:387:PRO:HD3	2.34	0.56
1:A:492:GLU:HG3	1:A:529:GLU:OE1	2.04	0.56
2:B:107:THR:O	2:B:188:TYR:HA	2.06	0.56
2:B:178:ILE:HG22	2:B:178:ILE:O	2.04	0.56
1:A:207:GLN:OE1	1:A:207:GLN:HA	2.06	0.56
2:B:62:ALA:HB1	2:B:71:TRP:CE3	2.41	0.56
2:B:382:ILE:HB	2:B:383:TRP:CZ3	2.40	0.56
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.71	0.56
2:B:333:GLY:N	2:B:336:GLN:HB2	2.20	0.56
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.41	0.56
1:A:233:GLU:N	1:A:240:THR:O	2.35	0.56
2:B:393:ILE:HG12	2:B:394:GLN:H	1.69	0.56
1:A:472:THR:OG1	1:A:477:THR:HG23	2.05	0.56
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.87	0.56
2:B:169:GLU:O	2:B:173:LYS:HG3	2.06	0.56
1:A:255:ASN:HA	1:A:258:GLN:OE1	2.05	0.56
2:B:128:THR:HB	2:B:146:TYR:HB2	1.87	0.56
2:B:210:LEU:HD13	2:B:216:THR:HA	1.87	0.56
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.74	0.55
2:B:38:CYS:O	2:B:47:ILE:HD11	2.06	0.55
2:B:41:MET:HB2	2:B:47:ILE:HG12	1.88	0.55
1:A:97:PRO:HD2	1:A:232:TYR:CZ	2.41	0.55
1:A:438:GLU:HG2	1:A:459:THR:HB	1.88	0.55
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:THR:HG22	2:B:299:ALA:H	1.71	0.55
2:B:421:PRO:HG2	2:B:424:LYS:HB2	1.88	0.55
1:A:68:SER:HB2	1:A:70:LYS:CE	2.37	0.55
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.42	0.55
2:B:253:THR:HA	2:B:291:GLU:O	2.07	0.55
2:B:115:TYR:HD1	2:B:115:TYR:H	1.50	0.55
1:A:442:VAL:HA	1:A:457:TYR:HB3	1.88	0.55
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.41	0.55
1:A:368:LEU:HD22	1:A:423:VAL:HG21	1.87	0.55
1:A:100:LEU:HB3	3:A:559:TBO:N1	2.22	0.55
1:A:31:ILE:HD13	1:A:133:PRO:O	2.07	0.55
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.42	0.55
2:B:177:ASP:O	2:B:179:VAL:HG23	2.07	0.55
2:B:198:HIS:O	2:B:201:LYS:HB3	2.06	0.55
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.88	0.54
2:B:229:TRP:C	2:B:231:GLY:H	2.13	0.54
2:B:380:ILE:HA	2:B:385:LYS:N	2.23	0.54
1:A:12:LEU:HD22	1:A:83:ARG:C	2.32	0.54
1:A:162:SER:O	1:A:165:THR:HB	2.08	0.54
1:A:271:TYR:HE1	1:A:314:VAL:H	1.55	0.54
2:B:12:LEU:HD23	2:B:83:ARG:O	2.07	0.54
2:B:59:PRO:HB2	2:B:76:ASP:CB	2.33	0.54
2:B:131:THR:HG23	2:B:143:ARG:HG3	1.90	0.54
2:B:320:ASP:OD1	2:B:322:SER:HB3	2.07	0.54
1:A:383:TRP:O	1:A:385:LYS:HG2	2.08	0.54
2:B:171:PHE:CE2	2:B:205:LEU:HA	2.42	0.54
2:B:398:TRP:C	2:B:400:THR:H	2.15	0.54
1:A:19:PRO:HA	1:A:83:ARG:HH12	1.73	0.54
2:B:78:ARG:NH1	2:B:412:PRO:O	2.41	0.54
2:B:378:GLU:O	2:B:382:ILE:HD12	2.07	0.54
1:A:46:LYS:HG3	1:A:148:VAL:HG11	1.90	0.54
1:A:101:LYS:NZ	1:A:321:PRO:HG2	2.23	0.54
1:A:537:PRO:HB2	1:A:540:LYS:HB2	1.89	0.54
2:B:253:THR:HB	2:B:256:ASP:CG	2.32	0.54
2:B:299:ALA:O	2:B:302:GLU:HB2	2.08	0.54
1:A:49:LYS:O	1:A:49:LYS:HG3	2.08	0.54
1:A:377:THR:O	1:A:381:VAL:HG23	2.07	0.54
2:B:393:ILE:O	2:B:416:PHE:HB3	2.08	0.54
1:A:372:VAL:O	1:A:375:ILE:HB	2.08	0.53
1:A:466:VAL:CG1	1:A:467:VAL:N	2.71	0.53
1:A:320:ASP:O	1:A:343:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HG13	1:A:389:PHE:CE2	2.43	0.53
2:B:338:THR:HG22	2:B:339:TYR:N	2.23	0.53
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.90	0.53
1:A:441:TYR:HA	1:A:496:VAL:HB	1.90	0.53
1:A:469:LEU:HB2	1:A:472:THR:HG21	1.91	0.53
2:B:115:TYR:C	2:B:117:SER:H	2.16	0.53
2:B:167:ILE:O	2:B:208:HIS:NE2	2.41	0.53
2:B:406:TRP:HZ2	2:B:410:TRP:O	1.92	0.53
1:A:111:VAL:HG22	1:A:187:LEU:HD12	1.90	0.53
1:A:426:TRP:CE3	1:A:426:TRP:HA	2.43	0.53
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.89	0.53
2:B:332:GLN:HB3	2:B:336:GLN:HB3	1.91	0.53
1:A:56:TYR:O	1:A:143:ARG:NH2	2.42	0.53
2:B:329:ILE:HD11	2:B:375:ILE:CD1	2.38	0.53
1:A:268:SER:HA	1:A:274:ILE:HD12	1.89	0.53
2:B:59:PRO:O	2:B:75:VAL:HG13	2.08	0.53
1:A:23:GLN:HE22	1:A:26:LEU:HD23	1.73	0.52
1:A:473:THR:HG22	1:A:475:GLN:H	1.73	0.52
2:B:325:LEU:H	2:B:325:LEU:HD23	1.73	0.52
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.74	0.52
1:A:486:LEU:HD11	1:A:521:ILE:HG23	1.90	0.52
2:B:330:GLN:HB2	2:B:332:GLN:NE2	2.24	0.52
1:A:207:GLN:O	1:A:210:LEU:HB3	2.10	0.52
1:A:340:GLN:HA	1:A:350:LYS:O	2.08	0.52
2:B:234:LEU:HD13	2:B:377:THR:HG21	1.91	0.52
1:A:420:PRO:CB	1:A:421:PRO:HD3	2.40	0.52
2:B:324:ASP:O	2:B:343:GLN:HG2	2.09	0.52
1:A:325:LEU:HD12	1:A:385:LYS:HB2	1.92	0.52
1:A:408:ALA:O	2:B:393:ILE:HG13	2.09	0.52
2:B:244:ILE:HG12	2:B:427:TYR:HB2	1.90	0.52
2:B:253:THR:HG23	2:B:289:LEU:O	2.10	0.52
2:B:253:THR:HG23	2:B:291:GLU:H	1.75	0.52
1:A:275:LYS:HB3	1:A:336:GLN:HE22	1.74	0.52
2:B:400:THR:O	2:B:400:THR:HG22	2.10	0.52
2:B:368:LEU:O	2:B:372:VAL:HG23	2.09	0.52
1:A:328:GLU:O	1:A:339:TYR:HA	2.10	0.52
1:A:116:PHE:O	1:A:148:VAL:HB	2.10	0.52
1:A:170:PRO:O	1:A:173:LYS:HB3	2.10	0.52
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.39	0.52
1:A:81:ASN:O	1:A:84:THR:HB	2.10	0.51
2:B:115:TYR:HB3	2:B:149:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:ILE:HB	2:B:383:TRP:CE3	2.45	0.51
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.08	0.51
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.26	0.51
1:A:40:GLU:O	1:A:44:GLU:N	2.44	0.51
1:A:101:LYS:HG2	1:A:319:TYR:HB3	1.92	0.51
1:A:408:ALA:HB1	2:B:364:ASP:CB	2.41	0.51
2:B:344:GLU:HB2	2:B:347:LYS:CB	2.38	0.51
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.45	0.51
1:A:10:VAL:HG21	1:A:153:TRP:CH2	2.46	0.51
1:A:458:VAL:HA	1:A:463:ARG:O	2.09	0.51
1:A:362:THR:HG22	1:A:363:ASN:H	1.75	0.50
1:A:365:VAL:HG22	1:A:423:VAL:HG12	1.93	0.50
2:B:111:VAL:N	2:B:185:ASP:O	2.43	0.50
2:B:285:GLY:HA3	2:B:287:LYS:HD2	1.92	0.50
1:A:195:ILE:HG23	1:A:199:ARG:HH12	1.76	0.50
1:A:317:VAL:HG23	1:A:349:LEU:CD1	2.37	0.50
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.27	0.50
1:A:500:GLN:O	1:A:503:LEU:HB3	2.11	0.50
1:A:505:ILE:HG22	1:A:506:ILE:N	2.26	0.50
1:A:103:LYS:O	1:A:236:PRO:HB2	2.10	0.50
1:A:245:VAL:O	1:A:247:PRO:HD3	2.11	0.50
1:A:439:THR:CG2	1:A:441:TYR:CE1	2.94	0.50
2:B:69:THR:HG22	2:B:70:LYS:N	2.27	0.50
1:A:188:TYR:HB3	3:A:559:TBO:H122	1.92	0.50
1:A:452:LEU:HD22	1:A:470:THR:HA	1.93	0.50
2:B:163:SER:C	2:B:167:ILE:HG12	2.36	0.50
2:B:99:GLY:O	2:B:102:LYS:HB2	2.11	0.50
1:A:153:TRP:CE3	1:A:156:SER:N	2.80	0.50
2:B:65:LYS:HB2	2:B:72:ARG:HG3	1.93	0.50
1:A:427:TYR:CZ	1:A:509:GLN:HA	2.47	0.50
2:B:74:LEU:C	2:B:74:LEU:HD23	2.37	0.50
2:B:156:SER:N	2:B:157:PRO:HD2	2.26	0.50
2:B:338:THR:HG22	2:B:339:TYR:H	1.76	0.50
1:A:153:TRP:HB3	1:A:156:SER:OG	2.12	0.49
1:A:394:GLN:HB3	1:A:397:THR:OG1	2.12	0.49
1:A:542:ILE:HG12	1:A:544:GLY:N	2.27	0.49
2:B:260:LEU:HD23	2:B:279:LEU:HD21	1.94	0.49
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.94	0.49
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.27	0.49
2:B:21:VAL:HG23	2:B:57:ASN:O	2.12	0.49
2:B:210:LEU:HD13	2:B:216:THR:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:SD	1:A:168:LEU:CD2	2.98	0.49
1:A:479:LEU:HA	1:A:482:ILE:CD1	2.40	0.49
2:B:239:TRP:HE3	2:B:350:LYS:HG3	1.78	0.49
2:B:320:ASP:H	2:B:343:GLN:HE22	1.60	0.49
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.20	0.49
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.47	0.49
1:A:194:GLU:O	1:A:195:ILE:C	2.55	0.49
1:A:387:PRO:HG2	1:A:389:PHE:CE1	2.47	0.49
2:B:246:LEU:HD11	2:B:307:ARG:HA	1.94	0.49
2:B:319:TYR:CE2	2:B:383:TRP:HD1	2.31	0.49
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.95	0.49
1:A:314:VAL:HG12	1:A:315:HIS:N	2.28	0.49
1:A:328:GLU:HA	1:A:390:LYS:HB2	1.95	0.49
1:A:442:VAL:CG2	1:A:485:ALA:HB2	2.43	0.49
2:B:47:ILE:HB	2:B:145:GLN:O	2.13	0.49
2:B:126:LYS:HA	2:B:145:GLN:NE2	2.27	0.49
2:B:50:ILE:HD12	2:B:143:ARG:HB3	1.94	0.49
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.48	0.49
2:B:308:GLU:HG3	2:B:311:LYS:HD2	1.94	0.49
1:A:33:ALA:O	1:A:37:ILE:HG13	2.13	0.49
1:A:224:GLU:C	1:A:226:PRO:HD2	2.37	0.49
2:B:178:ILE:CD1	2:B:191:SER:HB3	2.43	0.49
2:B:179:VAL:O	2:B:189:VAL:HA	2.12	0.49
2:B:255:ASN:O	2:B:258:GLN:HB2	2.12	0.49
1:A:59:PRO:O	1:A:75:VAL:HG13	2.12	0.49
1:A:257:ILE:O	1:A:261:VAL:HG23	2.13	0.49
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.94	0.49
2:B:263:LYS:HE2	2:B:425:LEU:CD1	2.35	0.49
2:B:268:SER:HA	2:B:274:ILE:CG2	2.43	0.49
2:B:320:ASP:O	2:B:343:GLN:OE1	2.31	0.49
1:A:495:ILE:HB	1:A:533:LEU:HD13	1.94	0.48
2:B:397:THR:O	2:B:401:TRP:HD1	1.95	0.48
1:A:19:PRO:HA	1:A:83:ARG:NH1	2.28	0.48
1:A:459:THR:CG2	1:A:463:ARG:HD2	2.44	0.48
2:B:128:THR:HG21	2:B:146:TYR:HB2	1.94	0.48
2:B:193:LEU:HD22	2:B:197:GLN:CB	2.43	0.48
1:A:105:SER:HB3	1:A:198:HIS:CG	2.48	0.48
1:A:438:GLU:CD	1:A:461:LYS:HD2	2.38	0.48
2:B:30:LYS:HG2	2:B:71:TRP:CZ3	2.48	0.48
2:B:391:LEU:HB2	2:B:416:PHE:CD2	2.47	0.48
2:B:340:GLN:HA	2:B:351:THR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PRO:CA	1:A:351:THR:HG21	2.29	0.48
2:B:86:ASP:O	2:B:89:GLU:HG2	2.13	0.48
2:B:254:VAL:HG23	2:B:291:GLU:HB3	1.96	0.48
2:B:325:LEU:CD2	2:B:387:PRO:HA	2.44	0.48
1:A:12:LEU:HD23	1:A:124:PHE:HZ	1.78	0.48
2:B:371:ALA:O	2:B:372:VAL:C	2.57	0.48
1:A:60:VAL:HA	1:A:75:VAL:CG2	2.29	0.48
1:A:468:PRO:O	1:A:469:LEU:HD23	2.14	0.48
1:A:474:ASN:H	1:A:474:ASN:ND2	2.11	0.48
1:A:486:LEU:HB3	1:A:524:GLN:OE1	2.13	0.48
1:A:553:SER:HA	1:A:556:ILE:O	2.13	0.48
2:B:254:VAL:HG12	2:B:258:GLN:HE21	1.79	0.48
2:B:363:ASN:O	2:B:364:ASP:C	2.56	0.48
2:B:35:VAL:CG2	2:B:36:GLU:N	2.76	0.48
2:B:88:TRP:CZ3	2:B:92:LEU:HD12	2.49	0.48
2:B:253:THR:CG2	2:B:289:LEU:O	2.62	0.48
2:B:326:ILE:HB	2:B:342:TYR:CE1	2.49	0.48
1:A:274:ILE:HA	1:A:306:ASN:OD1	2.14	0.47
1:A:341:ILE:HD12	1:A:350:LYS:O	2.14	0.47
1:A:441:TYR:CD1	1:A:441:TYR:N	2.82	0.47
1:A:519:ASN:O	1:A:522:ILE:HB	2.13	0.47
2:B:206:ARG:O	2:B:209:LEU:HB2	2.14	0.47
1:A:23:GLN:HG2	1:A:24:TRP:N	2.28	0.47
2:B:62:ALA:HB1	2:B:71:TRP:HE3	1.78	0.47
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.44	0.47
2:B:27:THR:CG2	2:B:30:LYS:HG3	2.45	0.47
2:B:178:ILE:HD12	2:B:189:VAL:HG12	1.95	0.47
1:A:246:LEU:HD21	1:A:310:LEU:HD13	1.97	0.47
1:A:522:ILE:HA	1:A:525:LEU:HD12	1.96	0.47
2:B:104:LYS:O	2:B:235:HIS:HA	2.14	0.47
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.50	0.47
2:B:164:MET:SD	2:B:168:LEU:CD1	3.01	0.47
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.15	0.47
1:A:34:LEU:HB3	1:A:132:ILE:HD13	1.97	0.47
1:A:433:PRO:HG2	2:B:290:THR:HG23	1.97	0.47
2:B:425:LEU:CD1	2:B:427:TYR:HB3	2.42	0.47
2:B:342:TYR:HB3	2:B:348:ASN:HB3	1.96	0.47
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.97	0.46
2:B:246:LEU:HD23	2:B:246:LEU:N	2.30	0.46
2:B:271:TYR:O	2:B:273:GLY:N	2.48	0.46
2:B:296:THR:HB	2:B:299:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLU:O	1:A:382:ILE:HG13	2.15	0.46
1:A:474:ASN:H	1:A:474:ASN:HD22	1.63	0.46
2:B:5:ILE:HG22	2:B:6:GLU:N	2.29	0.46
2:B:377:THR:O	2:B:378:GLU:C	2.58	0.46
1:A:447:ASN:HB3	1:A:450:THR:HG1	1.81	0.46
2:B:64:LYS:HE3	2:B:71:TRP:CZ2	2.50	0.46
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.33	0.46
2:B:320:ASP:N	2:B:343:GLN:HE22	2.13	0.46
1:A:13:LYS:HG3	1:A:83:ARG:O	2.16	0.46
1:A:77:PHE:CB	1:A:80:LEU:HD23	2.45	0.46
1:A:199:ARG:HB2	1:A:199:ARG:CZ	2.46	0.46
2:B:10:VAL:HG12	2:B:11:LYS:N	2.31	0.46
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.97	0.46
2:B:304:ALA:O	2:B:307:ARG:HB3	2.16	0.46
2:B:375:ILE:O	2:B:376:THR:C	2.58	0.46
1:A:47:ILE:HG22	1:A:48:SER:N	2.29	0.46
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.97	0.46
1:A:241:VAL:HG21	1:A:266:TRP:CZ2	2.51	0.46
1:A:412:PRO:O	1:A:414:TRP:HD1	1.99	0.46
2:B:65:LYS:HE3	2:B:407:GLN:HE21	1.81	0.46
2:B:116:PHE:HA	2:B:148:VAL:CG2	2.45	0.46
2:B:12:LEU:HD23	2:B:84:THR:HG23	1.98	0.46
2:B:303:LEU:HD11	2:B:307:ARG:NH2	2.30	0.46
1:A:12:LEU:HD22	1:A:83:ARG:O	2.15	0.46
1:A:373:GLN:HE22	2:B:397:THR:HA	1.76	0.46
1:A:406:TRP:CH2	2:B:417:VAL:O	2.69	0.46
1:A:442:VAL:HG12	1:A:481:ALA:HB1	1.98	0.46
2:B:380:ILE:O	2:B:381:VAL:C	2.59	0.46
1:A:420:PRO:HG2	1:A:421:PRO:HD3	1.98	0.46
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.51	0.46
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.98	0.46
1:A:87:PHE:O	2:B:55:PRO:HB3	2.16	0.46
1:A:153:TRP:CH2	1:A:155:GLY:HA3	2.51	0.46
1:A:329:ILE:HG23	1:A:338:THR:O	2.16	0.46
1:A:515:SER:O	1:A:516:GLU:C	2.59	0.46
1:A:194:GLU:HB2	1:A:197:GLN:HB3	1.98	0.45
1:A:547:GLN:HA	1:A:550:LYS:HB2	1.97	0.45
2:B:379:SER:O	2:B:383:TRP:HE3	1.98	0.45
1:A:375:ILE:HG21	1:A:389:PHE:CE2	2.50	0.45
2:B:296:THR:HG22	2:B:299:ALA:N	2.31	0.45
1:A:40:GLU:C	1:A:44:GLU:HG2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HD2	1:A:66:LYS:N	2.30	0.45
1:A:545:ASN:HA	1:A:548:VAL:CG2	2.47	0.45
2:B:103:LYS:HD2	2:B:191:SER:C	2.42	0.45
1:A:207:GLN:OE1	1:A:210:LEU:HD23	2.17	0.45
2:B:178:ILE:HG23	2:B:189:VAL:CG1	2.46	0.45
2:B:314:VAL:HG23	2:B:316:GLY:H	1.80	0.45
2:B:342:TYR:CD1	2:B:342:TYR:C	2.95	0.45
2:B:377:THR:HG22	2:B:381:VAL:CG2	2.46	0.45
1:A:244:ILE:HG22	1:A:310:LEU:HD11	1.97	0.45
1:A:283:LEU:O	1:A:285:GLY:N	2.50	0.45
1:A:341:ILE:HD12	1:A:341:ILE:N	2.32	0.45
1:A:365:VAL:O	1:A:368:LEU:HB3	2.17	0.45
1:A:484:LEU:O	1:A:485:ALA:C	2.59	0.45
2:B:375:ILE:HD12	2:B:389:PHE:HE1	1.81	0.45
1:A:168:LEU:HD23	1:A:209:LEU:HD21	1.99	0.45
1:A:317:VAL:O	1:A:349:LEU:HD12	2.17	0.45
1:A:318:TYR:CZ	3:A:559:TBO:H10	2.49	0.45
1:A:459:THR:HG21	1:A:463:ARG:HD2	1.98	0.45
2:B:78:ARG:O	2:B:82:LYS:HG3	2.17	0.45
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.30	0.45
2:B:373:GLN:NE2	2:B:406:TRP:CD2	2.84	0.45
1:A:106:VAL:O	1:A:107:THR:HB	2.17	0.45
1:A:418:ASN:O	1:A:419:THR:HG23	2.17	0.45
2:B:128:THR:CG2	2:B:146:TYR:HB2	2.46	0.45
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.82	0.45
1:A:376:THR:O	1:A:380:ILE:HG12	2.16	0.45
1:A:479:LEU:HD13	1:A:517:LEU:HG	1.97	0.45
2:B:253:THR:O	2:B:257:ILE:HG22	2.17	0.45
1:A:195:ILE:HG22	1:A:199:ARG:HH12	1.81	0.45
2:B:132:ILE:HG23	2:B:142:ILE:CB	2.42	0.45
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.30	0.45
1:A:178:ILE:HG23	1:A:190:GLY:O	2.16	0.45
1:A:296:THR:O	1:A:299:ALA:HB3	2.17	0.45
1:A:341:ILE:CD1	1:A:350:LYS:HB3	2.42	0.45
1:A:419:THR:CB	1:A:420:PRO:HD2	2.46	0.45
1:A:461:LYS:C	1:A:463:ARG:H	2.24	0.45
2:B:326:ILE:CD1	2:B:388:LYS:HE2	2.42	0.45
2:B:354:TYR:HE1	2:B:356:ARG:HD3	1.82	0.45
2:B:380:ILE:O	2:B:384:GLY:HA2	2.17	0.45
1:A:105:SER:HB3	1:A:198:HIS:ND1	2.32	0.44
1:A:127:TYR:C	1:A:129:ALA:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:O	1:A:176:PRO:HD3	2.17	0.44
2:B:170:PRO:HG2	2:B:171:PHE:H	1.82	0.44
2:B:234:LEU:CD1	2:B:377:THR:HG21	2.47	0.44
2:B:380:ILE:O	2:B:384:GLY:CA	2.65	0.44
1:A:260:LEU:HD23	1:A:279:LEU:HD13	1.98	0.44
1:A:532:TYR:CE2	2:B:289:LEU:HD13	2.52	0.44
2:B:303:LEU:O	2:B:307:ARG:HB2	2.17	0.44
2:B:417:VAL:C	2:B:419:THR:H	2.26	0.44
1:A:183:TYR:O	1:A:186:ASP:HB2	2.17	0.44
2:B:126:LYS:HA	2:B:145:GLN:HE21	1.81	0.44
2:B:191:SER:OG	2:B:198:HIS:ND1	2.50	0.44
2:B:257:ILE:CD1	2:B:282:LEU:HB3	2.47	0.44
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.99	0.44
1:A:479:LEU:CD1	1:A:517:LEU:HG	2.46	0.44
2:B:2:ILE:O	2:B:2:ILE:HG22	2.16	0.44
2:B:96:HIS:CE1	2:B:382:ILE:O	2.71	0.44
1:A:188:TYR:HD2	3:A:559:TBO:H71	1.82	0.44
2:B:410:TRP:O	2:B:410:TRP:CE3	2.70	0.44
1:A:142:ILE:O	1:A:142:ILE:HG13	2.18	0.44
1:A:511:ASP:HA	1:A:522:ILE:HD13	1.99	0.44
2:B:131:THR:OG1	2:B:143:ARG:NH1	2.43	0.44
2:B:209:LEU:O	2:B:215:THR:OG1	2.36	0.44
1:A:47:ILE:HG23	1:A:145:GLN:O	2.17	0.44
1:A:202:ILE:HG21	1:A:221:HIS:CB	2.47	0.44
2:B:21:VAL:CB	2:B:59:PRO:HD3	2.44	0.44
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.99	0.44
2:B:103:LYS:HD2	2:B:191:SER:CA	2.48	0.44
2:B:406:TRP:HH2	2:B:412:PRO:HD2	1.83	0.44
1:A:264:LEU:HD11	1:A:279:LEU:CD1	2.48	0.44
1:A:450:THR:O	1:A:452:LEU:HG	2.18	0.44
2:B:241:VAL:HG12	2:B:241:VAL:O	2.18	0.44
1:A:2:ILE:O	1:A:213:GLY:HA3	2.18	0.44
1:A:51:GLY:HA2	1:A:143:ARG:HD3	1.99	0.44
2:B:109:LEU:O	2:B:187:LEU:N	2.47	0.44
1:A:240:THR:HG22	1:A:315:HIS:HA	1.98	0.43
1:A:442:VAL:HG11	1:A:481:ALA:C	2.43	0.43
2:B:376:THR:HG22	2:B:380:ILE:HD11	2.00	0.43
1:A:373:GLN:O	1:A:376:THR:N	2.51	0.43
2:B:246:LEU:CD1	2:B:307:ARG:HA	2.48	0.43
2:B:401:TRP:O	2:B:404:GLU:HB3	2.18	0.43
1:A:101:LYS:HZ3	1:A:321:PRO:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HD22	1:A:156:SER:HA	1.99	0.43
1:A:259:LYS:O	1:A:263:LYS:HG3	2.18	0.43
1:A:457:TYR:CD1	1:A:457:TYR:C	2.96	0.43
2:B:125:ARG:NE	2:B:147:ASN:HA	2.30	0.43
2:B:188:TYR:CD1	2:B:188:TYR:N	2.86	0.43
1:A:465:LYS:O	1:A:466:VAL:HG23	2.17	0.43
2:B:63:ILE:O	2:B:72:ARG:N	2.51	0.43
2:B:163:SER:O	2:B:164:MET:C	2.61	0.43
2:B:171:PHE:CE2	2:B:205:LEU:CA	3.00	0.43
1:A:139:THR:HA	1:A:140:PRO:HD3	1.66	0.43
1:A:483:TYR:O	1:A:486:LEU:HB2	2.17	0.43
1:A:523:GLU:HA	1:A:526:ILE:HD12	1.99	0.43
2:B:60:VAL:HA	2:B:74:LEU:O	2.18	0.43
2:B:200:THR:C	2:B:202:ILE:N	2.73	0.43
2:B:329:ILE:CG2	2:B:330:GLN:N	2.82	0.43
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.53	0.43
1:A:521:ILE:HG22	1:A:525:LEU:HD11	1.99	0.43
1:A:532:TYR:HE2	2:B:289:LEU:HD13	1.83	0.43
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.19	0.43
2:B:308:GLU:C	2:B:310:LEU:N	2.75	0.43
2:B:349:LEU:H	2:B:349:LEU:HG	1.54	0.43
1:A:380:ILE:O	1:A:384:GLY:HA2	2.18	0.43
1:A:473:THR:HG22	1:A:474:ASN:N	2.34	0.43
2:B:81:ASN:HD22	2:B:154:LYS:HG3	1.82	0.43
1:A:397:THR:O	1:A:398:TRP:C	2.59	0.43
1:A:480:GLN:O	1:A:483:TYR:HB3	2.18	0.43
2:B:31:ILE:O	2:B:35:VAL:HG13	2.18	0.43
2:B:206:ARG:HA	2:B:209:LEU:HD12	2.00	0.43
1:A:178:ILE:CG2	1:A:189:VAL:HG12	2.49	0.43
1:A:368:LEU:O	1:A:372:VAL:HG23	2.18	0.43
1:A:426:TRP:HA	1:A:426:TRP:HE3	1.84	0.43
1:A:461:LYS:C	1:A:463:ARG:N	2.76	0.43
1:A:486:LEU:O	1:A:528:LYS:NZ	2.46	0.43
2:B:108:VAL:CG1	2:B:186:ASP:HB3	2.49	0.43
2:B:342:TYR:HB3	2:B:348:ASN:CB	2.49	0.43
2:B:354:TYR:CE1	2:B:356:ARG:HD3	2.53	0.43
1:A:155:GLY:O	1:A:156:SER:C	2.61	0.43
2:B:127:TYR:C	2:B:129:ALA:N	2.75	0.43
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.82	0.42
1:A:23:GLN:HG2	1:A:24:TRP:O	2.19	0.42
1:A:73:LYS:HG2	1:A:74:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLN:N	1:A:243:PRO:HD2	2.34	0.42
1:A:393:ILE:HG12	1:A:394:GLN:N	2.33	0.42
2:B:400:THR:C	2:B:401:TRP:CD1	2.97	0.42
1:A:68:SER:HB2	1:A:70:LYS:HE2	2.02	0.42
1:A:206:ARG:NH1	1:A:219:LYS:O	2.50	0.42
1:A:373:GLN:O	1:A:374:LYS:C	2.62	0.42
1:A:543:GLY:HA2	1:A:546:GLU:CB	2.42	0.42
2:B:377:THR:O	2:B:381:VAL:HG23	2.19	0.42
1:A:79:GLU:HG3	1:A:83:ARG:HH11	1.84	0.42
1:A:433:PRO:HA	1:A:532:TYR:CE2	2.54	0.42
2:B:100:LEU:HD11	2:B:190:GLY:HA3	2.01	0.42
2:B:255:ASN:O	2:B:259:LYS:HG3	2.19	0.42
1:A:210:LEU:O	1:A:210:LEU:HD12	2.19	0.42
2:B:377:THR:HA	2:B:380:ILE:HD12	2.02	0.42
1:A:293:ILE:HA	1:A:294:PRO:HD3	1.79	0.42
2:B:81:ASN:OD1	2:B:153:TRP:HD1	2.02	0.42
2:B:195:ILE:HD12	2:B:195:ILE:H	1.85	0.42
2:B:373:GLN:HA	2:B:376:THR:OG1	2.19	0.42
1:A:30:LYS:HD3	1:A:62:ALA:O	2.20	0.42
1:A:46:LYS:HE2	1:A:116:PHE:HB3	2.00	0.42
1:A:342:TYR:OH	1:A:390:LYS:HD2	2.19	0.42
1:A:477:THR:O	1:A:480:GLN:HB3	2.20	0.42
2:B:65:LYS:HD2	2:B:65:LYS:HA	1.80	0.42
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.75	0.42
2:B:132:ILE:HA	2:B:133:PRO:HD3	1.56	0.42
2:B:143:ARG:HG2	2:B:143:ARG:NH1	2.33	0.42
2:B:153:TRP:HE3	2:B:156:SER:OG	2.03	0.42
1:A:23:GLN:HB2	1:A:59:PRO:HB3	2.01	0.42
1:A:69:THR:H	1:A:70:LYS:HD3	1.84	0.42
1:A:171:PHE:CD1	1:A:205:LEU:HD13	2.54	0.42
1:A:229:TRP:O	1:A:232:TYR:N	2.52	0.42
2:B:52:PRO:C	2:B:54:ASN:N	2.77	0.42
2:B:134:SER:O	2:B:135:ILE:C	2.62	0.42
2:B:297:GLU:O	2:B:301:LEU:HD13	2.20	0.42
2:B:325:LEU:HG	2:B:387:PRO:HA	2.02	0.42
2:B:329:ILE:CG2	2:B:337:TRP:HE3	2.32	0.42
1:A:92:LEU:HD21	2:B:22:LYS:HD3	2.02	0.42
1:A:120:LEU:O	1:A:121:ASP:C	2.60	0.42
1:A:200:THR:O	1:A:204:GLU:HG3	2.20	0.42
1:A:543:GLY:CA	2:B:284:ARG:O	2.63	0.42
2:B:5:ILE:HD12	2:B:118:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.96	0.42
2:B:325:LEU:HG	2:B:387:PRO:CB	2.50	0.42
2:B:337:TRP:O	2:B:353:LYS:HG3	2.20	0.42
1:A:97:PRO:HG2	1:A:232:TYR:CG	2.54	0.42
1:A:235:HIS:O	1:A:237:ASP:N	2.53	0.42
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.55	0.42
1:A:510:PRO:O	1:A:511:ASP:HB3	2.20	0.42
2:B:27:THR:HG22	2:B:30:LYS:HG3	2.01	0.42
2:B:52:PRO:C	2:B:54:ASN:H	2.28	0.42
2:B:398:TRP:O	2:B:400:THR:N	2.53	0.42
1:A:169:GLU:O	1:A:170:PRO:C	2.60	0.42
2:B:65:LYS:CD	2:B:407:GLN:HG2	2.47	0.42
2:B:253:THR:H	2:B:256:ASP:HB2	1.85	0.42
1:A:68:SER:HB2	1:A:70:LYS:NZ	2.35	0.41
2:B:48:SER:O	2:B:145:GLN:N	2.52	0.41
2:B:111:VAL:O	2:B:115:TYR:HE1	2.02	0.41
1:A:191:SER:OG	1:A:198:HIS:CE1	2.73	0.41
1:A:276:VAL:HG12	1:A:276:VAL:O	2.20	0.41
1:A:391:LEU:HB2	1:A:414:TRP:CE3	2.54	0.41
2:B:20:LYS:HG3	2:B:56:TYR:HA	2.02	0.41
1:A:483:TYR:O	1:A:487:GLN:HG3	2.20	0.41
2:B:23:GLN:CG	2:B:133:PRO:HG3	2.47	0.41
2:B:110:ASP:HA	2:B:185:ASP:O	2.20	0.41
1:A:329:ILE:O	1:A:392:PRO:HG3	2.20	0.41
1:A:443:ASP:HB3	1:A:548:VAL:HB	2.00	0.41
1:A:524:GLN:O	1:A:528:LYS:HG3	2.21	0.41
2:B:27:THR:O	2:B:31:ILE:HG13	2.20	0.41
2:B:124:PHE:C	2:B:126:LYS:N	2.77	0.41
2:B:410:TRP:O	2:B:410:TRP:HE3	2.03	0.41
2:B:414:TRP:CD1	2:B:414:TRP:C	2.98	0.41
1:A:69:THR:N	1:A:70:LYS:HD3	2.36	0.41
1:A:149:LEU:HD13	1:A:156:SER:O	2.21	0.41
1:A:273:GLY:O	1:A:274:ILE:C	2.64	0.41
2:B:94:ILE:HA	2:B:95:PRO:HD3	1.81	0.41
2:B:162:SER:O	2:B:165:THR:HB	2.21	0.41
1:A:90:VAL:CG2	1:A:91:GLN:N	2.84	0.41
1:A:99:GLY:HA3	1:A:382:ILE:CG2	2.51	0.41
1:A:518:VAL:HA	1:A:521:ILE:HD12	2.02	0.41
1:A:205:LEU:O	1:A:208:HIS:HB3	2.21	0.41
1:A:440:PHE:CE2	1:A:459:THR:HG22	2.55	0.41
1:A:545:ASN:HA	1:A:548:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.56	0.41
2:B:264:LEU:HB3	2:B:274:ILE:HD11	2.03	0.41
2:B:329:ILE:HA	2:B:338:THR:O	2.20	0.41
2:B:330:GLN:O	2:B:338:THR:N	2.53	0.41
1:A:70:LYS:HD3	1:A:70:LYS:N	2.36	0.41
1:A:77:PHE:O	1:A:80:LEU:N	2.53	0.41
2:B:125:ARG:O	2:B:128:THR:N	2.54	0.41
2:B:216:THR:HA	2:B:217:PRO:HD3	1.80	0.41
2:B:239:TRP:CE3	2:B:350:LYS:HG3	2.54	0.41
2:B:269:GLN:OE1	2:B:269:GLN:HA	2.21	0.41
2:B:77:PHE:CD2	2:B:152:GLY:HA3	2.51	0.41
2:B:100:LEU:CD1	2:B:190:GLY:HA3	2.51	0.41
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.44	0.41
2:B:369:THR:CG2	2:B:370:GLU:N	2.83	0.41
1:A:99:GLY:HA2	1:A:383:TRP:HE1	1.81	0.41
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.51	0.41
2:B:79:GLU:O	2:B:80:LEU:C	2.63	0.41
2:B:181:CYS:N	2:B:188:TYR:O	2.53	0.41
2:B:398:TRP:C	2:B:400:THR:N	2.77	0.41
1:A:77:PHE:O	1:A:78:ARG:C	2.63	0.40
1:A:99:GLY:HA3	1:A:382:ILE:HG22	2.03	0.40
1:A:132:ILE:O	1:A:142:ILE:HG12	2.20	0.40
1:A:393:ILE:O	1:A:416:PHE:HB2	2.21	0.40
1:A:420:PRO:CG	1:A:421:PRO:HD3	2.51	0.40
2:B:33:ALA:O	2:B:36:GLU:HB2	2.20	0.40
2:B:210:LEU:HD12	2:B:214:LEU:HA	2.03	0.40
2:B:364:ASP:O	2:B:365:VAL:C	2.63	0.40
2:B:368:LEU:HD12	2:B:368:LEU:HA	1.90	0.40
2:B:370:GLU:O	2:B:371:ALA:C	2.63	0.40
2:B:96:HIS:CD2	2:B:384:GLY:HA3	2.56	0.40
2:B:160:PHE:O	2:B:161:GLN:C	2.63	0.40
2:B:161:GLN:O	2:B:162:SER:C	2.65	0.40
2:B:166:LYS:O	2:B:170:PRO:CD	2.66	0.40
2:B:193:LEU:HA	2:B:193:LEU:HD23	1.73	0.40
1:A:81:ASN:OD1	1:A:153:TRP:HA	2.22	0.40
1:A:90:VAL:CG2	1:A:91:GLN:H	2.30	0.40
2:B:125:ARG:O	2:B:126:LYS:C	2.64	0.40
1:A:225:PRO:N	1:A:226:PRO:HD2	2.37	0.40
1:A:229:TRP:O	1:A:230:MET:C	2.65	0.40
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.88	0.40
1:A:483:TYR:CE1	1:A:524:GLN:NE2	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:LYS:O	2:B:399:GLU:HG3	2.21	0.40
1:A:434:ILE:HG13	1:A:532:TYR:HB2	2.03	0.40
2:B:98:ALA:O	2:B:100:LEU:N	2.55	0.40
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.22	0.40
2:B:236:PRO:C	2:B:238:LYS:N	2.79	0.40
2:B:243:PRO:C	2:B:244:ILE:HG13	2.47	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	556/558 (100%)	415 (75%)	114 (20%)	27 (5%)	1	13
2	B	425/427 (100%)	309 (73%)	76 (18%)	40 (9%)	0	3
All	All	981/985 (100%)	724 (74%)	190 (19%)	67 (7%)	1	7

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	287	LYS
1	A	420	PRO
1	A	556	ILE
2	B	71	TRP
2	B	116	PHE
2	B	195	ILE
2	B	226	PRO
2	B	295	LEU
2	B	316	GLY
1	A	52	PRO
1	A	63	ILE

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Mol	Chain	Res	Type
1	A	67	ASP
1	A	90	VAL
1	A	274	ILE
1	A	284	ARG
1	A	462	GLY
2	B	2	ILE
2	B	4	PRO
2	B	45	GLY
2	B	93	GLY
2	B	99	GLY
2	B	162	SER
2	B	244	ILE
2	B	296	THR
2	B	372	VAL
1	A	134	SER
1	A	429	LEU
1	A	501	TYR
2	B	68	SER
2	B	213	GLY
2	B	273	GLY
2	B	317	VAL
2	B	359	GLY
1	A	114	ALA
1	A	135	ILE
1	A	169	GLU
1	A	236	PRO
2	B	122	GLU
2	B	128	THR
2	B	178	ILE
2	B	345	PRO
2	B	381	VAL
1	A	111	VAL
1	A	138	GLU
1	A	295	LEU
2	B	92	LEU
2	B	115	TYR
2	B	356	ARG
1	A	510	PRO
2	B	225	PRO
2	B	357	MET
2	B	358	ARG
2	B	363	ASN

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Mol	Chain	Res	Type
2	B	399	GLU
2	B	55	PRO
2	B	148	VAL
2	B	176	PRO
2	B	243	PRO
1	A	142	ILE
1	A	156	SER
1	A	294	PRO
2	B	314	VAL
2	B	421	PRO
1	A	276	VAL
2	B	217	PRO
1	A	505	ILE

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	453/498 (91%)	422 (93%)	31 (7%)	14	46
2	B	367/389 (94%)	317 (86%)	50 (14%)	3	18
All	All	820/887 (92%)	739 (90%)	81 (10%)	7	31

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ILE
1	A	60	VAL
1	A	69	THR
1	A	73	LYS
1	A	78	ARG
1	A	80	LEU
1	A	94	ILE
1	A	97	PRO
1	A	109	LEU
1	A	124	PHE

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Mol	Chain	Res	Type
1	A	172	LYS
1	A	199	ARG
1	A	242	GLN
1	A	296	THR
1	A	310	LEU
1	A	338	THR
1	A	340	GLN
1	A	341	ILE
1	A	344	GLU
1	A	351	THR
1	A	362	THR
1	A	393	ILE
1	A	411	ILE
1	A	422	LEU
1	A	423	VAL
1	A	426	TRP
1	A	482	ILE
1	A	505	ILE
1	A	529	GLU
1	A	540	LYS
1	A	542	ILE
2	B	6	GLU
2	B	12	LEU
2	B	20	LYS
2	B	21	VAL
2	B	26	LEU
2	B	35	VAL
2	B	46	LYS
2	B	49	LYS
2	B	50	ILE
2	B	60	VAL
2	B	63	ILE
2	B	70	LYS
2	B	88	TRP
2	B	91	GLN
2	B	132	ILE
2	B	139	THR
2	B	164	MET
2	B	178	ILE
2	B	185	ASP
2	B	194	GLU
2	B	205	LEU

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Mol	Chain	Res	Type
2	B	240	THR
2	B	246	LEU
2	B	250	ASP
2	B	257	ILE
2	B	266	TRP
2	B	274	ILE
2	B	283	LEU
2	B	287	LYS
2	B	290	THR
2	B	293	ILE
2	B	301	LEU
2	B	315	HIS
2	B	317	VAL
2	B	318	TYR
2	B	325	LEU
2	B	330	GLN
2	B	332	GLN
2	B	341	ILE
2	B	345	PRO
2	B	356	ARG
2	B	369	THR
2	B	378	GLU
2	B	386	THR
2	B	407	GLN
2	B	410	TRP
2	B	413	GLU
2	B	421	PRO
2	B	425	LEU
2	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	145	GLN
1	A	147	ASN
1	A	182	GLN
1	A	197	GLN
1	A	255	ASN
1	A	269	GLN
1	A	334	GLN
1	A	336	GLN

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Mol	Chain	Res	Type
1	A	367	GLN
1	A	373	GLN
1	A	407	GLN
1	A	471	ASN
1	A	474	ASN
1	A	480	GLN
1	A	539	HIS
2	B	96	HIS
2	B	137	ASN
2	B	161	GLN
2	B	207	GLN
2	B	255	ASN
2	B	315	HIS
2	B	332	GLN
2	B	340	GLN
2	B	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	TBO	A	559	-	22,23,23	2.53	7 (31%)	19,34,34	3.27	9 (47%)

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	TBO	A	559	-	-	1/5/17/17	0/2/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	559	TBO	C2-N1	8.17	1.43	1.36
3	A	559	TBO	C10-C9	4.12	1.45	1.38
3	A	559	TBO	C7-N6	-2.98	1.43	1.47
3	A	559	TBO	C1A-N1	2.80	1.43	1.38
3	A	559	TBO	C4-N3	-2.67	1.44	1.46
3	A	559	TBO	C12-N6	2.51	1.51	1.47
3	A	559	TBO	C8-C7A	2.43	1.43	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	559	TBO	C3A-N3-C2	-7.55	106.47	109.95
3	A	559	TBO	C16-C14-C15	7.19	131.14	114.59
3	A	559	TBO	C15-C14-C13	-5.49	106.17	122.66
3	A	559	TBO	C1A-N1-C2	-4.96	106.97	110.67
3	A	559	TBO	C12-N6-C7	3.62	118.38	112.07
3	A	559	TBO	C10-C1A-C3A	-2.66	118.19	121.46
3	A	559	TBO	C12-C13-C14	2.36	131.03	127.12
3	A	559	TBO	C10-C1A-N1	2.31	135.49	130.83
3	A	559	TBO	C9-C8-C7A	-2.08	119.84	122.53

There are no chirality outliers.

All (1) torsion outliers are listed below:

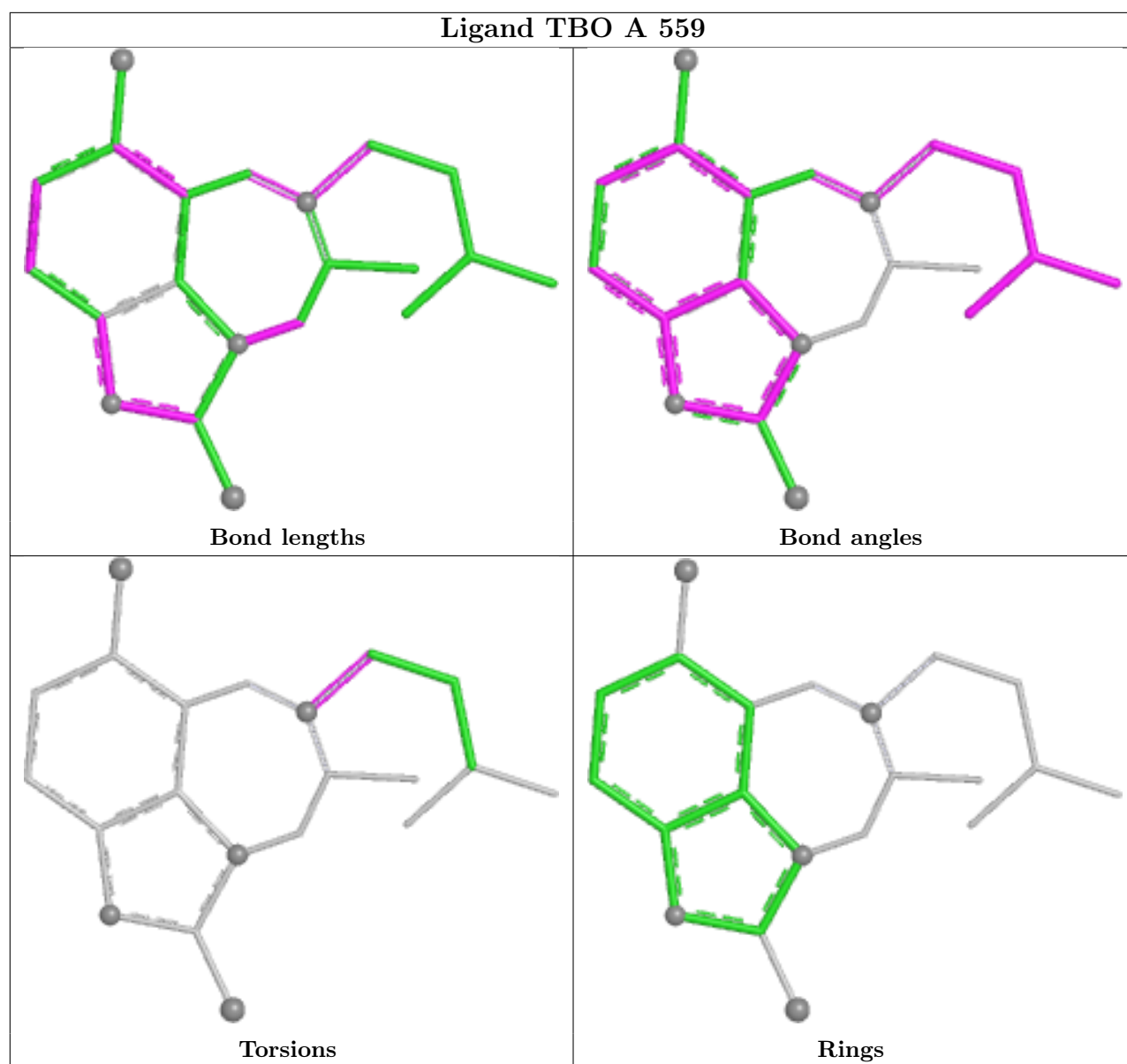
Mol	Chain	Res	Type	Atoms
3	A	559	TBO	C13-C12-N6-C5

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	559	TBO	8	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 [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	558/558 (100%)	-0.04	7 (1%) 75 55	22, 71, 97, 100	0
2	B	427/427 (100%)	-0.10	4 (0%) 81 64	18, 59, 97, 100	0
All	All	985/985 (100%)	-0.06	11 (1%) 78 61	18, 68, 97, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	316	GLY	3.0
1	A	253	THR	3.0
2	B	94	ILE	2.9
1	A	434	ILE	2.8
1	A	26	LEU	2.7
2	B	228	LEU	2.6
1	A	66	LYS	2.3
2	B	95	PRO	2.3
1	A	264	LEU	2.2
1	A	547	GLN	2.1
1	A	554	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

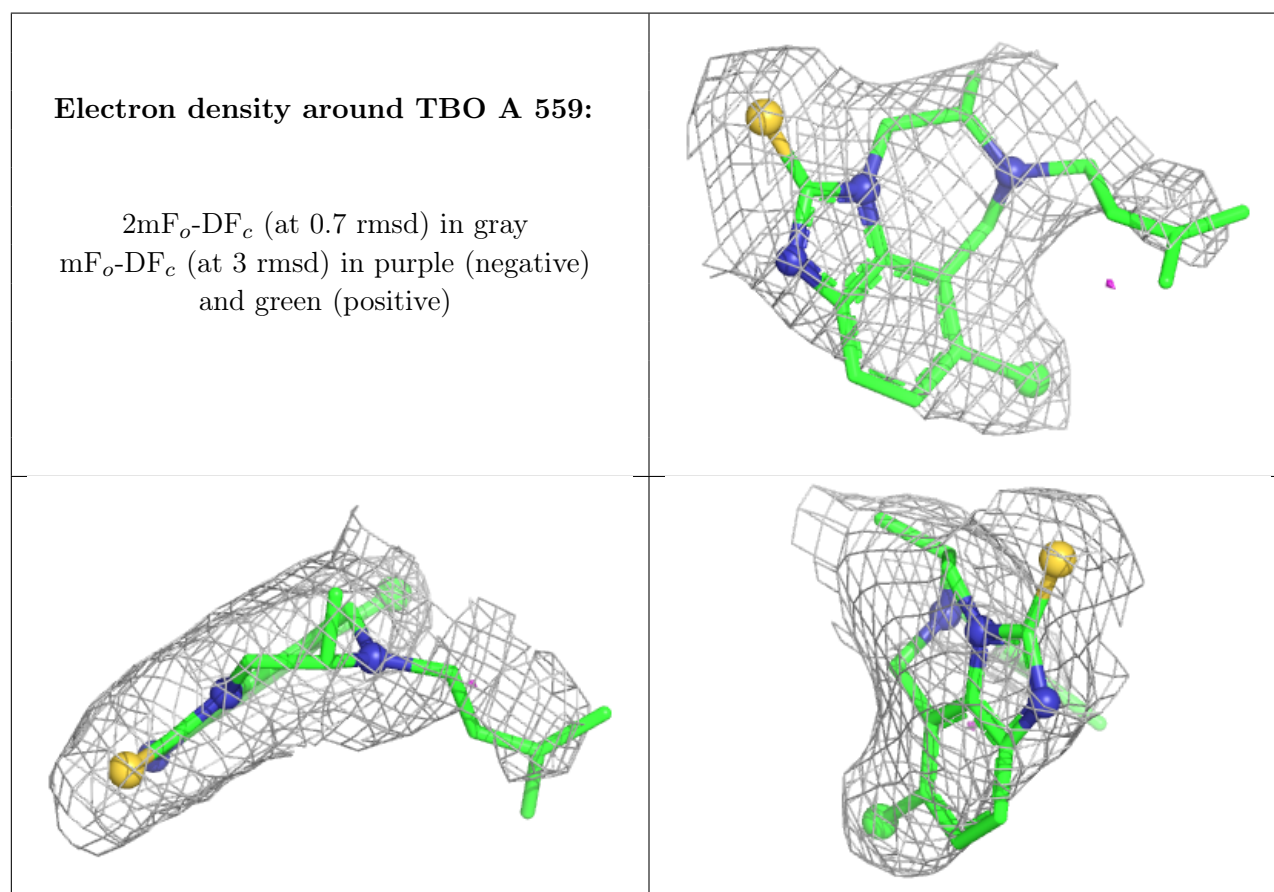
There are no oligosaccharides in this entry.

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	TBO	A	559	21/21	0.95	0.10	59,67,70,73	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.