



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:17 PM UTC

PDB ID : 1S1W / pdb_00001s1w
Title : Crystal structure of V106A mutant HIV-1 reverse transcriptase in complex with UC-781
Authors : Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Stammers, D.K.
Deposited on : 2004-01-07
Resolution : 2.70 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

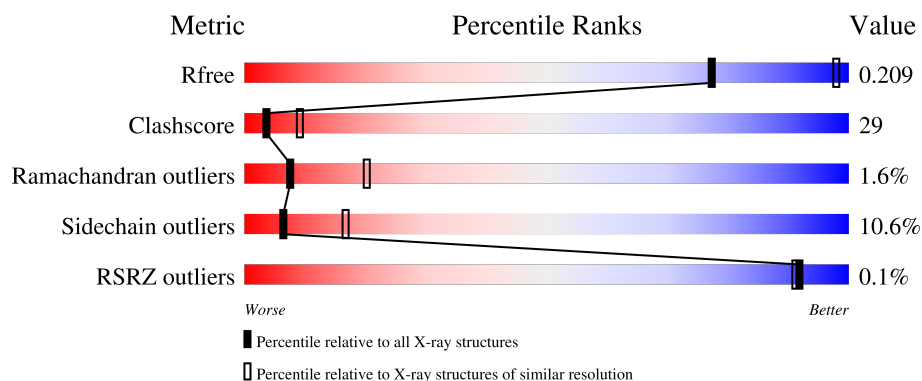
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

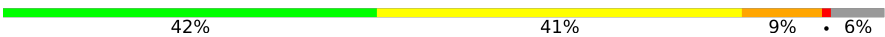
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7740 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	525	Total	C	N	O	S	0	0	0
			4308	2790	714	796	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	ALA	VAL	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

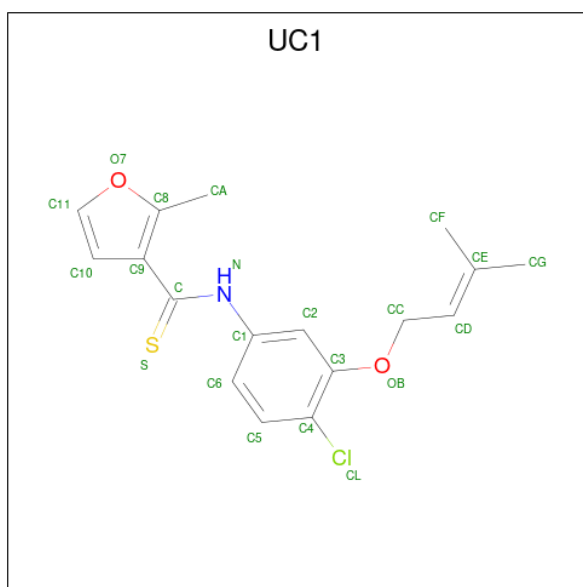
- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3344	2184	549	604	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	ALA	VAL	engineered mutation	UNP P04585

- Molecule 3 is 2-METHYL-FURAN-3-CARBOTHIOIC ACID [4-CHLORO-3-(3-METHYLBUT-2-ENYLOXY)-PHENYL]-AMIDE (CCD ID: UC1) (formula: C₁₇H₁₈ClNO₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			22	17	1	1	2	1		

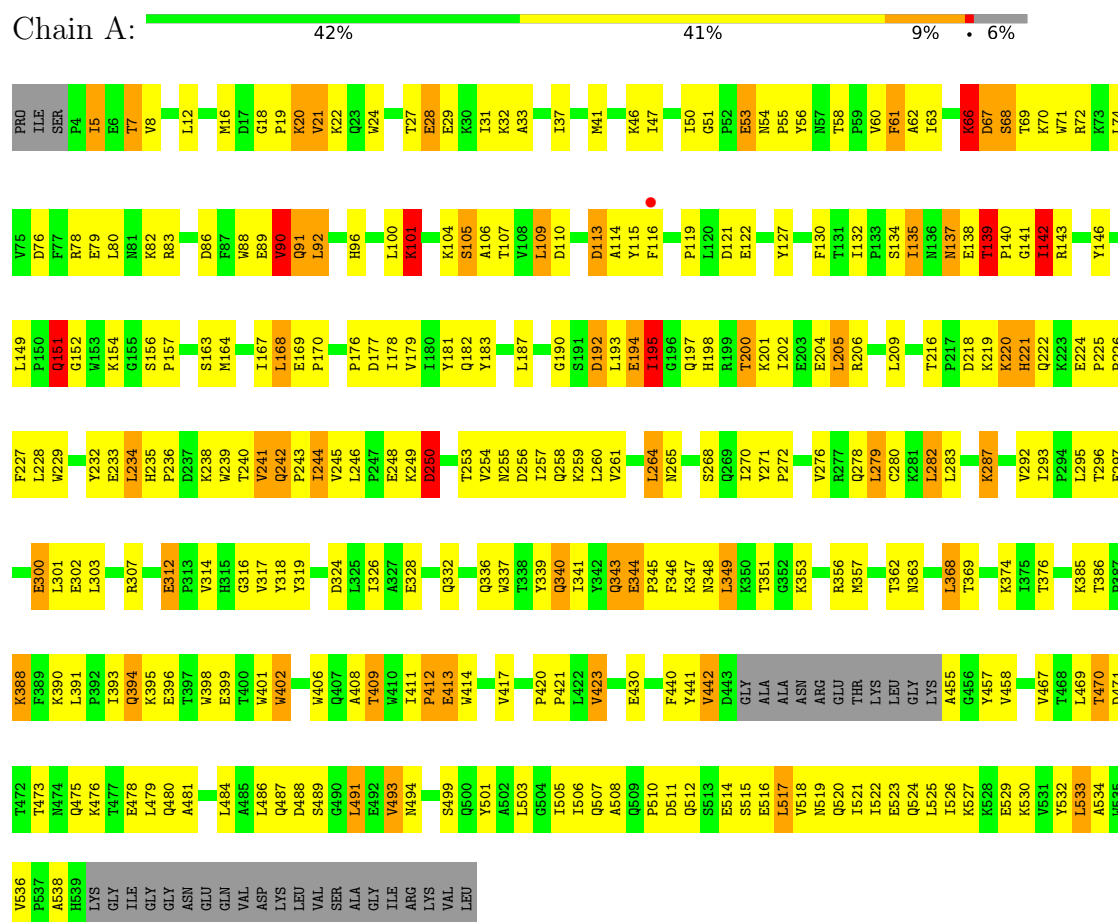
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	17	Total	O	0	0
			17	17		

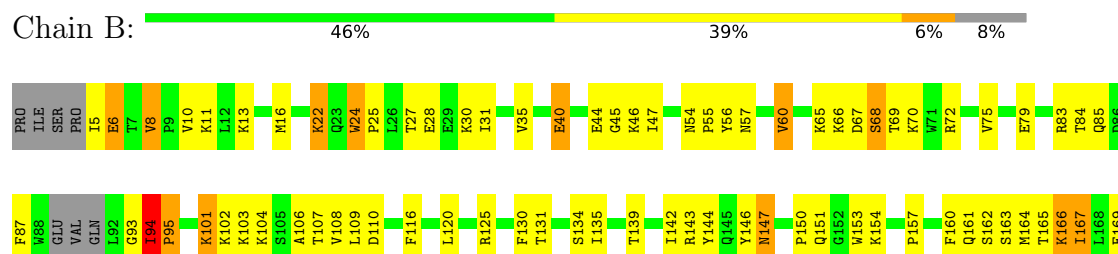
3 Residue-property plots

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



M418	K331	L234	P170
T419	G332	H235	R171
P420	G333	P236	R172
L421	Q334	D237	K173
L422	G335	K238	Q174
V423	Q336	W239	N175
K424	W337	V240	P176
L425	T338	T241	D177
W426	Y339	Q242	I178
Y427	Y342	P243	V179
Q428	Q343	L244	I180
LEU		D250	Y183
GLU		S251	M184
LYS	K346	K347	D185
GLU	K347	W252	D186
PRO	N348	T253	L187
ILE	L349	V254	Y188
VAL	K350	Q258	
GLY	T351		S191
ALA	G352	V261	D192
GLU	Y354		L193
THR	K353		E194
PHE	A355	W266	I195
	ARG	Q269	G196
	MET	I270	
	ARG		R199
	GLY	L274	
	ALA	K275	K200
	HIS	D276	T201
	T362	V276	L202
	R363	R277	E203
	D364		E204
	V365	C280	L205
	K366	K281	R206
	G367	L282	Q207
	L368	L283	H208
	T369	R284	
	E370	G285	L209
	A371	T286	L210
	V372	K287	G213
	Q373	A288	LEU
	K374	L289	THR
		E291	PRO
		V292	ASP
			LYS
		L295	LYS
		T296	HIS
			GLN
		L303	LYS
			LYS
		N306	GLU
			P225
		P313	P226
			F227
		L325	W228
			M230
		E328	G231
	W401	I329	Y232
		C330	F233
	V417		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.54Å 114.69Å 65.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 2.70 29.74 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.74-2.70) 97.1 (29.74-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.206 , 0.280 0.198 , 0.209	Depositor DCC
R_{free} test set	1359 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7740	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, UC1

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	0.65	0/4415	1.12	30/6002 (0.5%)
2	B	0.61	0/3441	1.09	19/4675 (0.4%)
All	All	0.63	0/7856	1.10	49/10677 (0.5%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	THR	CA-C-N	12.42	132.57	119.90
1	A	139	THR	C-N-CA	12.42	132.57	119.90
1	A	140	PRO	N-CA-C	10.45	127.66	111.15
1	A	67	ASP	N-CA-C	9.69	125.37	113.17
1	A	349	LEU	N-CA-C	-9.09	100.60	112.68
2	B	94	ILE	CA-C-N	8.35	130.28	119.84
2	B	94	ILE	C-N-CA	8.35	130.28	119.84
1	A	241	VAL	N-CA-C	-7.98	98.54	109.55
1	A	234	LEU	N-CA-C	7.87	121.08	108.41
1	A	141	GLY	N-CA-C	7.81	131.69	113.18
2	B	229	TRP	CA-CB-CG	-7.45	99.44	113.60
2	B	417	VAL	N-CA-C	7.22	119.35	108.80
2	B	147	ASN	N-CA-C	-6.56	105.81	113.88
1	A	343	GLN	N-CA-C	-6.39	104.43	112.93
2	B	87	PHE	N-CA-C	6.39	119.21	108.02
1	A	90	VAL	N-CA-C	-6.15	103.26	110.21
2	B	139	THR	CA-C-N	6.06	127.41	119.84
2	B	139	THR	C-N-CA	6.06	127.41	119.84
2	B	56	TYR	N-CA-C	5.93	118.56	110.55
1	A	192	ASP	N-CA-C	-5.87	104.78	112.41
2	B	231	GLY	N-CA-C	-5.79	99.45	113.18
1	A	488	ASP	N-CA-C	5.76	118.50	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLU	N-CA-C	-5.74	104.94	111.14
1	A	348	ASN	N-CA-C	5.74	118.66	110.10
2	B	381	VAL	N-CA-C	5.72	116.46	110.62
1	A	96	HIS	N-CA-C	-5.71	102.58	109.72
2	B	186	ASP	N-CA-C	5.67	119.31	110.17
1	A	250	ASP	N-CA-C	-5.67	106.35	113.72
1	A	494	ASN	N-CA-C	-5.67	99.17	108.41
1	A	244	ILE	N-CA-C	5.66	116.29	107.28
1	A	21	VAL	N-CA-C	5.65	116.02	108.11
1	A	66	LYS	N-CA-C	5.64	122.82	110.80
1	A	142	ILE	N-CA-C	5.64	116.33	108.89
1	A	68	SER	N-CA-C	5.62	118.63	109.24
2	B	68	SER	N-CA-C	-5.58	98.91	110.80
1	A	221	HIS	N-CA-C	5.48	119.66	112.92
2	B	343	GLN	N-CA-C	-5.47	107.61	114.56
1	A	388	LYS	N-CA-C	-5.44	101.11	109.76
2	B	401	TRP	N-CA-C	5.42	120.91	113.97
2	B	24	TRP	CA-C-N	5.40	125.71	119.93
2	B	24	TRP	C-N-CA	5.40	125.71	119.93
1	A	101	LYS	N-CA-C	-5.37	100.94	109.59
1	A	344	GLU	N-CA-C	-5.28	101.97	109.62
1	A	8	VAL	CB-CA-C	-5.19	104.82	110.78
1	A	82	LYS	N-CA-C	-5.15	106.26	112.54
2	B	201	LYS	N-CA-C	-5.14	105.79	111.71
2	B	209	LEU	N-CA-C	-5.14	106.70	113.12
1	A	151	GLN	N-CA-C	-5.06	102.89	110.23
1	A	71	TRP	N-CA-C	5.05	117.72	109.59

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	4308	0	4339	261	0
2	B	3344	0	3368	198	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	0	18	1	0
4	A	49	0	0	3	0
4	B	17	0	0	3	0
All	All	7740	0	7725	451	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 29.

All (451) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:PHE:CB	2:B:231:GLY:HA2	1.74	1.16
2:B:227:PHE:HB3	2:B:231:GLY:CA	1.78	1.12
1:A:242:GLN:HB2	1:A:243:PRO:HD2	1.34	1.08
2:B:167:ILE:HD11	2:B:209:LEU:HD23	1.37	1.03
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.02	1.02
1:A:27:THR:HG22	1:A:29:GLU:H	1.24	1.02
1:A:395:LYS:H	1:A:395:LYS:HD2	1.23	1.00
2:B:353:LYS:NZ	2:B:428:GLN:HG3	1.76	1.00
1:A:195:ILE:HD13	1:A:195:ILE:H	1.27	0.97
2:B:166:LYS:HE3	2:B:166:LYS:HA	1.46	0.96
2:B:5:ILE:HG22	2:B:6:GLU:H	1.30	0.93
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.52	0.91
1:A:206:ARG:NH1	1:A:218:ASP:HA	1.85	0.91
1:A:249:LYS:HZ3	1:A:256:ASP:CG	1.79	0.90
2:B:230:MET:C	2:B:232:TYR:H	1.77	0.87
2:B:172:ARG:O	2:B:176:PRO:HG3	1.74	0.86
2:B:353:LYS:HZ3	2:B:428:GLN:HG3	1.41	0.83
2:B:206:ARG:NH2	2:B:227:PHE:CG	2.46	0.83
1:A:242:GLN:HB2	1:A:243:PRO:CD	2.08	0.83
2:B:93:GLY:O	2:B:95:PRO:HD3	1.79	0.83
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.43	0.82
2:B:175:ASN:ND2	2:B:201:LYS:HD3	1.94	0.82
1:A:61:PHE:CE2	1:A:74:LEU:HB3	2.15	0.81
2:B:379:SER:OG	2:B:387:PRO:HG3	1.80	0.81
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.47	0.80
1:A:195:ILE:HD13	1:A:195:ILE:N	1.96	0.79
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.63	0.79
1:A:89:GLU:OE1	1:A:92:LEU:HB2	1.81	0.78
1:A:135:ILE:H	1:A:135:ILE:HD12	1.48	0.78
1:A:388:LYS:HG2	1:A:413:GLU:OE1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:HB3	2:B:428:GLN:HE22	1.49	0.77
1:A:279:LEU:HA	1:A:282:LEU:HD22	1.67	0.77
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.66	0.77
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.20	0.76
2:B:229:TRP:HA	2:B:229:TRP:CE3	2.18	0.76
2:B:353:LYS:HZ2	2:B:428:GLN:HG3	1.47	0.76
1:A:206:ARG:HH12	1:A:218:ASP:HA	1.50	0.75
1:A:260:LEU:HG	1:A:264:LEU:HD22	1.69	0.75
2:B:142:ILE:H	2:B:142:ILE:HD12	1.52	0.74
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.67	0.74
2:B:227:PHE:CB	2:B:231:GLY:CA	2.52	0.74
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.69	0.74
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.70	0.74
1:A:151:GLN:C	1:A:151:GLN:HE21	1.96	0.74
1:A:63:ILE:HD13	1:A:74:LEU:HB2	1.69	0.73
2:B:169:GLU:HG2	2:B:170:PRO:HD3	1.71	0.73
2:B:154:LYS:O	2:B:157:PRO:HD2	1.89	0.73
1:A:151:GLN:HE21	1:A:152:GLY:N	1.86	0.73
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.71	0.72
2:B:151:GLN:HB3	2:B:185:ASP:OD1	1.89	0.72
2:B:66:LYS:CG	2:B:230:MET:HA	2.20	0.71
1:A:61:PHE:CD1	1:A:63:ILE:HD11	2.26	0.71
1:A:218:ASP:OD2	1:A:220:LYS:HB2	1.90	0.71
1:A:200:THR:HG22	1:A:201:LYS:N	2.04	0.70
2:B:229:TRP:HZ2	2:B:373:GLN:OE1	1.74	0.70
1:A:395:LYS:HD2	1:A:395:LYS:N	2.02	0.70
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.72	0.70
2:B:206:ARG:NH2	2:B:227:PHE:CD2	2.58	0.70
2:B:175:ASN:N	2:B:176:PRO:HD3	2.07	0.70
1:A:27:THR:HG22	1:A:29:GLU:N	2.03	0.70
2:B:169:GLU:N	2:B:170:PRO:HD2	2.07	0.70
2:B:284:ARG:O	2:B:287:LYS:NZ	2.24	0.70
1:A:195:ILE:H	1:A:195:ILE:CD1	2.04	0.69
2:B:69:THR:HG23	2:B:70:LYS:HZ2	1.58	0.69
2:B:175:ASN:HD21	2:B:201:LYS:HD3	1.58	0.68
1:A:58:THR:HG23	1:A:76:ASP:O	1.94	0.68
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.28	0.68
1:A:28:GLU:HG3	1:A:135:ILE:HG22	1.75	0.67
2:B:103:LYS:O	2:B:236:PRO:HG2	1.94	0.67
2:B:201:LYS:HE3	2:B:201:LYS:HA	1.76	0.67
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:HA	1:A:511:ASP:CG	2.19	0.67
2:B:5:ILE:HG22	2:B:6:GLU:N	2.08	0.66
2:B:266:TRP:O	2:B:269:GLN:HG2	1.95	0.66
2:B:230:MET:HB2	2:B:232:TYR:HB2	1.78	0.66
1:A:151:GLN:NE2	1:A:152:GLY:N	2.44	0.66
2:B:202:ILE:HG21	2:B:227:PHE:CZ	2.31	0.66
2:B:195:ILE:O	2:B:199:ARG:HG3	1.96	0.66
2:B:167:ILE:HG13	2:B:167:ILE:O	1.94	0.66
2:B:420:PRO:O	2:B:423:VAL:HG12	1.95	0.65
2:B:40:GLU:O	2:B:44:GLU:HG3	1.96	0.65
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.32	0.65
1:A:76:ASP:OD2	1:A:78:ARG:HG3	1.97	0.65
2:B:103:LYS:HE2	2:B:179:VAL:CG2	2.26	0.65
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.79	0.65
2:B:66:LYS:HG2	2:B:230:MET:HA	1.77	0.64
1:A:524:GLN:HA	1:A:524:GLN:OE1	1.96	0.64
2:B:207:GLN:HA	2:B:210:LEU:HB2	1.79	0.64
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.33	0.64
1:A:413:GLU:HA	4:A:1034:HOH:O	1.97	0.63
2:B:22:LYS:HD3	4:B:1052:HOH:O	1.97	0.63
2:B:229:TRP:CZ2	2:B:373:GLN:OE1	2.51	0.63
2:B:163:SER:O	2:B:167:ILE:HG22	1.97	0.63
2:B:169:GLU:CG	2:B:170:PRO:HD3	2.29	0.63
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.80	0.63
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.32	0.63
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.79	0.63
2:B:295:LEU:N	2:B:295:LEU:HD12	2.13	0.63
2:B:69:THR:HG23	2:B:70:LYS:NZ	2.13	0.63
2:B:106:ALA:O	2:B:234:LEU:HB2	2.00	0.62
1:A:61:PHE:N	1:A:61:PHE:CD2	2.66	0.62
1:A:167:ILE:O	1:A:170:PRO:HD2	1.99	0.62
1:A:411:ILE:O	1:A:412:PRO:O	2.17	0.62
1:A:105:SER:HB2	1:A:198:HIS:CG	2.35	0.61
2:B:108:VAL:C	2:B:109:LEU:HD12	2.25	0.61
1:A:62:ALA:C	1:A:63:ILE:HD12	2.27	0.60
1:A:218:ASP:O	1:A:222:GLN:HG3	2.01	0.60
1:A:491:LEU:O	1:A:529:GLU:HB2	2.01	0.60
2:B:107:THR:HG21	2:B:227:PHE:CE1	2.37	0.60
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.36	0.60
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.37	0.59
2:B:109:LEU:HD11	2:B:227:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HD11	2:B:233:GLU:HG2	1.84	0.59
1:A:255:ASN:O	1:A:259:LYS:HD3	2.02	0.59
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.85	0.59
1:A:134:SER:OG	1:A:139:THR:O	2.16	0.59
1:A:236:PRO:HA	3:A:999:UC1:H5	1.83	0.59
1:A:249:LYS:NZ	1:A:256:ASP:CG	2.57	0.59
1:A:374:LYS:HG2	4:A:1031:HOH:O	2.03	0.59
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.83	0.59
1:A:270:ILE:O	1:A:272:PRO:HD3	2.03	0.59
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.01	0.59
2:B:142:ILE:HD12	2:B:142:ILE:N	2.18	0.59
1:A:61:PHE:N	1:A:61:PHE:HD2	2.01	0.58
1:A:163:SER:O	1:A:167:ILE:HG13	2.03	0.58
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.85	0.58
1:A:5:ILE:HD12	1:A:119:PRO:HD2	1.85	0.58
1:A:61:PHE:CE1	1:A:63:ILE:HD11	2.39	0.58
2:B:109:LEU:HD11	2:B:227:PHE:HE1	1.66	0.58
1:A:398:TRP:NE1	1:A:411:ILE:HD12	2.17	0.58
1:A:72:ARG:HH11	1:A:72:ARG:HG2	1.69	0.58
1:A:104:LYS:NZ	1:A:104:LYS:HB3	2.18	0.58
2:B:428:GLN:HG2	2:B:428:GLN:O	2.04	0.58
1:A:369:THR:HG21	1:A:409:THR:HG21	1.86	0.57
2:B:202:ILE:HG21	2:B:227:PHE:HZ	1.69	0.57
1:A:523:GLU:O	1:A:527:LYS:HG2	2.04	0.57
1:A:101:LYS:HE3	1:A:101:LYS:N	2.19	0.57
1:A:135:ILE:HD12	1:A:135:ILE:N	2.17	0.57
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.37	0.57
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.03	0.57
1:A:200:THR:CG2	1:A:201:LYS:N	2.67	0.57
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.68	0.57
1:A:135:ILE:H	1:A:135:ILE:CD1	2.07	0.56
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.40	0.56
1:A:28:GLU:OE1	1:A:31:ILE:HD12	2.05	0.56
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.41	0.56
2:B:167:ILE:CD1	2:B:209:LEU:HD23	2.26	0.56
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.88	0.56
1:A:249:LYS:NZ	1:A:256:ASP:OD2	2.38	0.56
2:B:173:LYS:C	2:B:176:PRO:HD3	2.31	0.56
1:A:194:GLU:HG2	1:A:197:GLN:HB2	1.88	0.56
2:B:173:LYS:O	2:B:176:PRO:HD3	2.06	0.55
2:B:203:GLU:O	2:B:206:ARG:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:MET:C	2:B:232:TYR:N	2.49	0.55
1:A:319:TYR:HA	1:A:349:LEU:HD21	1.87	0.55
2:B:13:LYS:HB2	2:B:16:MET:SD	2.45	0.55
2:B:227:PHE:HB3	2:B:231:GLY:C	2.30	0.55
1:A:368:LEU:HD13	1:A:368:LEU:C	2.31	0.55
1:A:376:THR:HG23	1:A:386:THR:HG22	1.88	0.55
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.37	0.55
1:A:137:ASN:O	1:A:139:THR:N	2.40	0.55
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.88	0.55
2:B:160:PHE:CE1	2:B:164:MET:HE2	2.41	0.55
1:A:61:PHE:CZ	1:A:74:LEU:HD23	2.41	0.55
1:A:107:THR:HG22	1:A:109:LEU:HD13	1.87	0.55
2:B:66:LYS:HG2	2:B:230:MET:HG3	1.89	0.55
2:B:173:LYS:HA	2:B:176:PRO:CG	2.37	0.55
1:A:480:GLN:HA	1:A:480:GLN:OE1	2.08	0.54
1:A:69:THR:O	1:A:69:THR:HG22	2.07	0.54
1:A:257:ILE:O	1:A:261:VAL:HG23	2.06	0.54
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.43	0.54
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.43	0.54
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.43	0.54
1:A:254:VAL:O	1:A:258:GLN:HG3	2.08	0.54
1:A:328:GLU:O	1:A:339:TYR:HA	2.08	0.54
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.43	0.54
1:A:28:GLU:CG	1:A:135:ILE:HG22	2.37	0.54
1:A:478:GLU:OE2	1:A:499:SER:OG	2.25	0.54
2:B:5:ILE:CG2	2:B:6:GLU:H	2.12	0.54
1:A:61:PHE:CZ	1:A:74:LEU:HB3	2.43	0.53
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.44	0.53
1:A:24:TRP:HZ3	1:A:61:PHE:HB3	1.73	0.53
1:A:27:THR:CG2	1:A:29:GLU:HB3	2.38	0.53
1:A:72:ARG:HG2	1:A:72:ARG:NH1	2.22	0.53
2:B:94:ILE:HG13	2:B:94:ILE:O	2.08	0.53
2:B:104:LYS:HA	2:B:237:ASP:HB2	1.90	0.53
2:B:332:GLN:HB3	2:B:428:GLN:NE2	2.20	0.53
2:B:169:GLU:HG2	2:B:170:PRO:CD	2.38	0.53
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.44	0.53
1:A:142:ILE:N	1:A:142:ILE:HD13	2.24	0.52
1:A:241:VAL:O	1:A:242:GLN:O	2.27	0.52
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.44	0.52
2:B:380:ILE:O	2:B:384:GLY:N	2.42	0.52
1:A:56:TYR:O	1:A:143:ARG:NH2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:C	1:A:139:THR:H	2.18	0.52
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.10	0.52
2:B:172:ARG:NH2	2:B:180:ILE:O	2.42	0.52
1:A:518:VAL:O	1:A:522:ILE:HG13	2.10	0.52
2:B:103:LYS:HD3	2:B:192:ASP:OD1	2.10	0.52
1:A:51:GLY:C	1:A:53:GLU:H	2.17	0.51
1:A:63:ILE:CD1	1:A:74:LEU:HB2	2.37	0.51
1:A:340:GLN:HA	1:A:351:THR:HA	1.92	0.51
1:A:481:ALA:O	1:A:484:LEU:HB2	2.11	0.51
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.41	0.51
2:B:230:MET:HE3	2:B:232:TYR:HD1	1.75	0.51
2:B:161:GLN:HE21	2:B:165:THR:HG23	1.76	0.51
2:B:101:LYS:O	2:B:236:PRO:HB2	2.10	0.51
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.46	0.51
2:B:374:LYS:NZ	4:B:1064:HOH:O	2.44	0.51
1:A:18:GLY:HA3	1:A:127:TYR:CD1	2.46	0.51
1:A:100:LEU:HD12	1:A:318:TYR:CE1	2.45	0.50
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.40	0.50
2:B:169:GLU:N	2:B:170:PRO:CD	2.73	0.50
1:A:279:LEU:HD22	1:A:302:GLU:OE1	2.12	0.50
2:B:79:GLU:O	2:B:83:ARG:HG3	2.11	0.50
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.93	0.50
2:B:169:GLU:CG	2:B:170:PRO:CD	2.89	0.50
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.47	0.50
1:A:86:ASP:HA	1:A:154:LYS:HZ1	1.77	0.50
1:A:395:LYS:H	1:A:395:LYS:CD	1.96	0.49
1:A:244:ILE:O	1:A:244:ILE:HG23	2.12	0.49
1:A:268:SER:CB	1:A:353:LYS:HE2	2.42	0.49
1:A:18:GLY:HA3	1:A:127:TYR:HD1	1.77	0.49
1:A:63:ILE:HD12	1:A:63:ILE:N	2.27	0.49
2:B:254:VAL:O	2:B:258:GLN:HG3	2.12	0.49
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.94	0.49
2:B:186:ASP:OD1	2:B:228:LEU:HD12	2.13	0.49
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.94	0.49
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.95	0.49
2:B:194:GLU:HG3	2:B:196:GLY:H	1.78	0.49
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.13	0.49
2:B:160:PHE:O	2:B:160:PHE:CD1	2.65	0.49
2:B:200:THR:O	2:B:204:GLU:HG3	2.13	0.49
2:B:241:VAL:HG11	2:B:313:PRO:HG3	1.95	0.49
1:A:100:LEU:HD12	1:A:318:TYR:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HA	1:A:226:PRO:C	2.37	0.49
1:A:507:GLN:HE22	2:B:421:PRO:HB3	1.77	0.49
1:A:476:LYS:CD	1:A:517:LEU:HD12	2.43	0.49
2:B:173:LYS:CA	2:B:176:PRO:HG3	2.41	0.49
2:B:350:LYS:HG3	2:B:351:THR:H	1.76	0.49
1:A:357:MET:HE2	1:A:512:GLN:HE21	1.78	0.48
1:A:486:LEU:HD12	1:A:521:ILE:HG23	1.95	0.48
2:B:125:ARG:HH11	2:B:147:ASN:HD22	1.61	0.48
1:A:205:LEU:HD22	1:A:209:LEU:HG	1.94	0.48
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.48	0.48
1:A:104:LYS:HB3	1:A:104:LYS:HZ2	1.78	0.48
1:A:253:THR:O	1:A:254:VAL:C	2.56	0.48
2:B:353:LYS:HZ3	2:B:428:GLN:CG	2.19	0.48
2:B:195:ILE:HD11	2:B:233:GLU:CG	2.43	0.48
1:A:279:LEU:CA	1:A:282:LEU:HD22	2.42	0.48
1:A:420:PRO:HA	1:A:421:PRO:C	2.37	0.48
1:A:455:ALA:HB3	1:A:467:VAL:O	2.13	0.48
2:B:366:LYS:O	2:B:370:GLU:HG3	2.14	0.48
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.13	0.48
1:A:357:MET:SD	1:A:514:GLU:OE1	2.72	0.48
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.49	0.48
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.96	0.48
1:A:522:ILE:O	1:A:526:ILE:HG13	2.15	0.47
2:B:195:ILE:HD11	2:B:233:GLU:CD	2.38	0.47
2:B:206:ARG:NH2	2:B:227:PHE:CD1	2.80	0.47
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.39	0.47
1:A:60:VAL:HG21	1:A:130:PHE:CD1	2.50	0.47
1:A:229:TRP:O	1:A:232:TYR:HD1	1.97	0.47
1:A:264:LEU:HB3	1:A:276:VAL:CG1	2.44	0.47
1:A:200:THR:HG22	1:A:201:LYS:H	1.80	0.47
1:A:295:LEU:HD12	1:A:300:GLU:CD	2.39	0.47
1:A:506:ILE:HG21	1:A:533:LEU:HD12	1.95	0.47
1:A:68:SER:C	1:A:70:LYS:H	2.23	0.47
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.29	0.47
1:A:507:GLN:NE2	2:B:421:PRO:HB3	2.30	0.47
1:A:202:ILE:O	1:A:206:ARG:HG3	2.15	0.47
2:B:142:ILE:H	2:B:142:ILE:CD1	2.24	0.47
2:B:125:ARG:NH1	2:B:147:ASN:HD22	2.13	0.47
1:A:346:PHE:N	1:A:346:PHE:CD1	2.82	0.46
2:B:332:GLN:HB2	2:B:336:GLN:O	2.15	0.46
1:A:268:SER:HB3	1:A:353:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:HD2	2:B:67:ASP:H	1.79	0.46
1:A:110:ASP:O	1:A:216:THR:HG22	2.15	0.46
1:A:151:GLN:HE21	1:A:151:GLN:CA	2.26	0.46
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.97	0.46
1:A:295:LEU:HD12	1:A:300:GLU:OE2	2.16	0.46
1:A:470:THR:O	1:A:471:ASP:HB2	2.16	0.46
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.23	0.46
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.41	0.46
2:B:350:LYS:HG3	2:B:351:THR:N	2.30	0.46
1:A:121:ASP:O	1:A:122:GLU:C	2.59	0.46
1:A:193:LEU:HB3	1:A:197:GLN:HG3	1.97	0.46
1:A:430:GLU:CG	1:A:530:LYS:HB3	2.46	0.46
2:B:166:LYS:HA	2:B:166:LYS:CE	2.26	0.46
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.98	0.46
1:A:115:TYR:HB3	1:A:149:LEU:HB2	1.98	0.46
1:A:194:GLU:HG2	1:A:197:GLN:CB	2.45	0.46
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.98	0.46
2:B:11:LYS:O	2:B:85:GLN:HB3	2.16	0.46
2:B:66:LYS:HD2	2:B:67:ASP:N	2.31	0.46
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.51	0.46
1:A:24:TRP:CZ3	1:A:61:PHE:HB3	2.50	0.46
1:A:106:ALA:HB1	1:A:227:PHE:HE2	1.80	0.46
1:A:401:TRP:HH2	1:A:508:ALA:O	1.98	0.46
1:A:515:SER:O	1:A:519:ASN:ND2	2.49	0.46
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.98	0.45
1:A:374:LYS:HD3	1:A:374:LYS:C	2.42	0.45
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.50	0.45
2:B:276:VAL:O	2:B:277:ARG:C	2.59	0.45
1:A:137:ASN:C	1:A:139:THR:N	2.73	0.45
2:B:24:TRP:CG	2:B:25:PRO:HD2	2.50	0.45
1:A:105:SER:O	1:A:190:GLY:HA2	2.16	0.45
1:A:279:LEU:HA	1:A:282:LEU:CD2	2.41	0.45
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.51	0.45
2:B:227:PHE:C	2:B:231:GLY:HA2	2.41	0.45
2:B:350:LYS:CG	2:B:351:THR:N	2.79	0.45
1:A:218:ASP:O	1:A:219:LYS:C	2.60	0.45
1:A:324:ASP:O	1:A:343:GLN:HG2	2.16	0.45
1:A:28:GLU:OE1	1:A:135:ILE:HG22	2.17	0.45
1:A:178:ILE:HG22	1:A:179:VAL:N	2.30	0.45
1:A:90:VAL:O	1:A:92:LEU:N	2.50	0.45
1:A:233:GLU:HB3	1:A:240:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:OD2	1:A:250:ASP:N	2.46	0.45
1:A:391:LEU:C	1:A:417:VAL:HG12	2.41	0.45
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.52	0.45
2:B:85:GLN:O	2:B:85:GLN:HG3	2.16	0.45
1:A:72:ARG:NH1	1:A:74:LEU:HD12	2.31	0.45
1:A:287:LYS:NZ	4:A:1026:HOH:O	2.46	0.45
2:B:241:VAL:HG13	2:B:351:THR:OG1	2.16	0.45
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.17	0.45
1:A:88:TRP:HB2	2:B:54:ASN:O	2.17	0.45
2:B:45:GLY:HA2	4:B:1056:HOH:O	2.17	0.45
2:B:380:ILE:O	2:B:384:GLY:HA2	2.17	0.45
2:B:229:TRP:HZ2	2:B:373:GLN:CD	2.26	0.44
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.99	0.44
2:B:110:ASP:HB2	2:B:228:LEU:HG	1.99	0.44
2:B:205:LEU:HD23	2:B:208:HIS:HB3	1.99	0.44
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.53	0.44
2:B:93:GLY:C	2:B:95:PRO:HD3	2.41	0.44
2:B:104:LYS:O	2:B:235:HIS:HA	2.17	0.44
1:A:20:LYS:HD2	1:A:55:PRO:O	2.17	0.44
2:B:229:TRP:CZ2	2:B:373:GLN:CD	2.95	0.44
2:B:425:LEU:HD22	2:B:426:TRP:CD1	2.52	0.44
1:A:268:SER:OG	1:A:353:LYS:HE2	2.18	0.44
1:A:279:LEU:O	1:A:282:LEU:HB2	2.18	0.44
2:B:205:LEU:HD22	2:B:209:LEU:HG	1.99	0.44
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.53	0.44
1:A:28:GLU:O	1:A:32:LYS:HG3	2.18	0.44
1:A:50:ILE:HD12	1:A:54:ASN:CB	2.47	0.44
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.33	0.44
2:B:103:LYS:HD2	2:B:191:SER:CA	2.48	0.44
1:A:536:VAL:HG12	2:B:258:GLN:HB3	2.00	0.44
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.53	0.44
2:B:365:VAL:O	2:B:369:THR:HG23	2.18	0.44
1:A:101:LYS:N	1:A:101:LYS:CE	2.81	0.44
1:A:312:GLU:O	1:A:312:GLU:HG2	2.18	0.44
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.52	0.43
1:A:193:LEU:HD13	1:A:197:GLN:HG3	1.99	0.43
2:B:328:GLU:O	2:B:339:TYR:HA	2.18	0.43
2:B:423:VAL:HG13	2:B:424:LYS:N	2.32	0.43
1:A:33:ALA:O	1:A:37:ILE:HG13	2.18	0.43
1:A:226:PRO:HA	1:A:234:LEU:O	2.18	0.43
2:B:8:VAL:O	2:B:8:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ILE:O	2:B:35:VAL:HG23	2.18	0.43
2:B:295:LEU:N	2:B:295:LEU:CD1	2.81	0.43
1:A:27:THR:HG21	1:A:29:GLU:HB3	1.99	0.43
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.99	0.43
1:A:417:VAL:O	1:A:417:VAL:HG13	2.18	0.43
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.54	0.43
1:A:516:GLU:O	1:A:519:ASN:N	2.51	0.43
2:B:24:TRP:CE2	2:B:399:GLU:HB3	2.53	0.43
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.53	0.43
1:A:115:TYR:HD1	1:A:151:GLN:HA	1.84	0.43
1:A:248:GLU:HG3	1:A:248:GLU:O	2.19	0.43
1:A:394:GLN:H	1:A:394:GLN:HG2	1.57	0.43
1:A:67:ASP:O	1:A:67:ASP:CG	2.62	0.43
1:A:259:LYS:N	1:A:259:LYS:HD2	2.33	0.43
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.51	0.43
1:A:409:THR:O	2:B:364:ASP:HB2	2.19	0.43
1:A:505:ILE:O	1:A:510:PRO:HD3	2.18	0.43
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.01	0.43
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.88	0.43
1:A:332:GLN:HB3	1:A:336:GLN:HB3	2.01	0.43
2:B:84:THR:HB	2:B:154:LYS:HE2	2.00	0.43
1:A:228:LEU:HA	1:A:232:TYR:O	2.19	0.42
2:B:202:ILE:HG21	2:B:227:PHE:CE1	2.53	0.42
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.01	0.42
2:B:102:LYS:O	2:B:103:LYS:C	2.62	0.42
1:A:176:PRO:C	1:A:178:ILE:H	2.26	0.42
1:A:218:ASP:OD1	1:A:221:HIS:ND1	2.53	0.42
2:B:227:PHE:HB2	2:B:231:GLY:HA2	1.85	0.42
1:A:51:GLY:C	1:A:53:GLU:N	2.78	0.42
2:B:253:THR:HA	2:B:292:VAL:HA	2.01	0.42
1:A:393:ILE:O	1:A:414:TRP:CZ3	2.72	0.42
2:B:22:LYS:HE3	2:B:22:LYS:HB2	1.88	0.42
2:B:161:GLN:O	2:B:164:MET:HB3	2.20	0.42
1:A:5:ILE:H	1:A:5:ILE:HG13	1.73	0.42
1:A:487:GLN:HA	1:A:524:GLN:NE2	2.35	0.42
2:B:103:LYS:HD2	2:B:191:SER:HA	2.02	0.42
1:A:27:THR:HG22	1:A:29:GLU:HB3	2.00	0.42
1:A:198:HIS:C	1:A:200:THR:N	2.78	0.42
2:B:60:VAL:HG11	2:B:130:PHE:CD1	2.54	0.42
2:B:160:PHE:HE1	2:B:164:MET:HE2	1.83	0.42
2:B:230:MET:HB2	2:B:230:MET:HE2	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.90	0.42
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.35	0.42
1:A:317:VAL:HG22	1:A:318:TYR:H	1.85	0.42
1:A:525:LEU:HD23	1:A:525:LEU:HA	1.92	0.41
1:A:169:GLU:O	1:A:170:PRO:C	2.63	0.41
1:A:517:LEU:HD23	1:A:520:GLN:HE21	1.85	0.41
1:A:115:TYR:N	1:A:115:TYR:CD2	2.89	0.41
1:A:194:GLU:O	1:A:197:GLN:N	2.54	0.41
1:A:271:TYR:CE1	1:A:314:VAL:HG13	2.54	0.41
1:A:278:GLN:NE2	1:A:278:GLN:HA	2.36	0.41
1:A:457:TYR:CD1	1:A:457:TYR:C	2.97	0.41
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.55	0.41
2:B:335:GLY:O	2:B:355:ALA:HA	2.21	0.41
1:A:164:MET:HG3	1:A:168:LEU:HD22	2.03	0.41
1:A:344:GLU:O	1:A:347:LYS:HB2	2.21	0.41
2:B:70:LYS:HA	2:B:70:LYS:HD3	1.85	0.41
2:B:171:PHE:O	2:B:175:ASN:HB2	2.20	0.41
2:B:242:GLN:O	2:B:242:GLN:HG3	2.21	0.41
1:A:110:ASP:O	1:A:216:THR:HA	2.20	0.41
1:A:24:TRP:HZ3	1:A:61:PHE:CG	2.38	0.41
1:A:66:LYS:HA	1:A:66:LYS:HD3	1.91	0.41
1:A:337:TRP:CH2	1:A:368:LEU:HB2	2.56	0.41
1:A:37:ILE:O	1:A:41:MET:HG3	2.20	0.41
1:A:46:LYS:NZ	1:A:113:ASP:OD2	2.54	0.41
1:A:486:LEU:HA	1:A:486:LEU:HD23	1.89	0.41
1:A:489:SER:CB	1:A:493:VAL:CG1	2.99	0.41
1:A:224:GLU:OE2	1:A:225:PRO:HD2	2.21	0.41
1:A:293:ILE:N	1:A:293:ILE:HD12	2.36	0.41
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.68	0.41
2:B:175:ASN:H	2:B:176:PRO:HD3	1.81	0.41
1:A:228:LEU:HD23	1:A:233:GLU:HA	2.03	0.41
1:A:245:VAL:HG13	1:A:245:VAL:O	2.21	0.41
1:A:264:LEU:HB3	1:A:276:VAL:HG11	2.02	0.41
2:B:425:LEU:C	2:B:425:LEU:HD23	2.46	0.41
1:A:134:SER:CB	1:A:139:THR:O	2.69	0.40
1:A:7:THR:HG21	1:A:121:ASP:HA	2.03	0.40
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.50	0.40
1:A:116:PHE:CZ	1:A:151:GLN:HB2	2.57	0.40
1:A:132:ILE:HB	1:A:142:ILE:CG1	2.50	0.40
1:A:235:HIS:HB2	1:A:238:LYS:O	2.20	0.40
1:A:326:ILE:O	1:A:341:ILE:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:N	2:B:176:PRO:CD	2.80	0.40
2:B:227:PHE:HB2	2:B:231:GLY:CA	2.46	0.40
1:A:19:PRO:CD	1:A:80:LEU:HD13	2.52	0.40
1:A:151:GLN:NE2	1:A:151:GLN:CA	2.84	0.40
1:A:401:TRP:CH2	1:A:508:ALA:O	2.75	0.40
1:A:441:TYR:CD1	2:B:286:THR:HG22	2.56	0.40
2:B:46:LYS:CE	2:B:116:PHE:HB3	2.52	0.40
2:B:287:LYS:HD3	2:B:291:GLU:OE2	2.20	0.40
2:B:422:LEU:O	2:B:425:LEU:HB3	2.22	0.40
1:A:296:THR:O	1:A:297:GLU:C	2.64	0.40
2:B:10:VAL:HG11	2:B:153:TRP:CZ2	2.57	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	520/560 (93%)	476 (92%)	34 (6%)	10 (2%)	6	17
2	B	396/440 (90%)	357 (90%)	34 (9%)	5 (1%)	9	25
All	All	916/1000 (92%)	833 (91%)	68 (7%)	15 (2%)	7	20

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	91	GLN
1	A	137	ASN
1	A	195	ILE
1	A	242	GLN
1	A	412	PRO
1	A	538	ALA

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Mol	Chain	Res	Type
2	B	232	TYR
1	A	114	ALA
1	A	138	GLU
2	B	250	ASP
2	B	95	PRO
2	B	162	SER
1	A	345	PRO
2	B	334	GLN

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	472/498 (95%)	414 (88%)	58 (12%)	4	12
2	B	367/399 (92%)	336 (92%)	31 (8%)	10	26
All	All	839/897 (94%)	750 (89%)	89 (11%)	6	17

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	20	LYS
1	A	21	VAL
1	A	22	LYS
1	A	28	GLU
1	A	53	GLU
1	A	61	PHE
1	A	90	VAL
1	A	91	GLN
1	A	92	LEU
1	A	101	LYS
1	A	105	SER
1	A	109	LEU
1	A	113	ASP

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Mol	Chain	Res	Type
1	A	135	ILE
1	A	139	THR
1	A	142	ILE
1	A	151	GLN
1	A	168	LEU
1	A	177	ASP
1	A	182	GLN
1	A	194	GLU
1	A	195	ILE
1	A	200	THR
1	A	205	LEU
1	A	220	LYS
1	A	250	ASP
1	A	264	LEU
1	A	265	ASN
1	A	279	LEU
1	A	282	LEU
1	A	283	LEU
1	A	287	LYS
1	A	300	GLU
1	A	301	LEU
1	A	303	LEU
1	A	312	GLU
1	A	340	GLN
1	A	356	ARG
1	A	362	THR
1	A	368	LEU
1	A	394	GLN
1	A	396	GLU
1	A	402	TRP
1	A	409	THR
1	A	413	GLU
1	A	423	VAL
1	A	442	VAL
1	A	458	VAL
1	A	470	THR
1	A	473	THR
1	A	479	LEU
1	A	491	LEU
1	A	493	VAL
1	A	503	LEU
1	A	517	LEU

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Mol	Chain	Res	Type
1	A	533	LEU
2	B	6	GLU
2	B	8	VAL
2	B	22	LYS
2	B	40	GLU
2	B	55	PRO
2	B	60	VAL
2	B	72	ARG
2	B	94	ILE
2	B	101	LYS
2	B	134	SER
2	B	166	LYS
2	B	167	ILE
2	B	173	LYS
2	B	175	ASN
2	B	178	ILE
2	B	201	LYS
2	B	205	LEU
2	B	210	LEU
2	B	225	PRO
2	B	230	MET
2	B	233	GLU
2	B	240	THR
2	B	250	ASP
2	B	280	CYS
2	B	283	LEU
2	B	286	THR
2	B	289	LEU
2	B	295	LEU
2	B	303	LEU
2	B	368	LEU
2	B	388	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	151	GLN
1	A	197	GLN
1	A	208	HIS
1	A	222	GLN
1	A	235	HIS

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Mol	Chain	Res	Type
1	A	242	GLN
1	A	255	ASN
1	A	258	GLN
1	A	278	GLN
1	A	407	GLN
1	A	475	GLN
1	A	487	GLN
1	A	507	GLN
1	A	509	GLN
1	A	512	GLN
1	A	520	GLN
2	B	57	ASN
2	B	147	ASN
2	B	207	GLN
2	B	208	HIS
2	B	242	GLN
2	B	258	GLN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	336	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	1.27	1 (25%)	1,8,10	7.01	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	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	2.14	1.49	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	7.01	118.51	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	UC1	A	999	-	22,23,23	2.11	6 (27%)	26,31,31	1.28	4 (15%)

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	UC1	A	999	-	-	3/12/14/14	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	UC1	C-N	7.27	1.42	1.34
3	A	999	UC1	O7-C8	2.98	1.39	1.36
3	A	999	UC1	C9-C8	-2.22	1.33	1.36
3	A	999	UC1	C10-C9	2.19	1.50	1.43
3	A	999	UC1	C2-C3	2.05	1.42	1.38
3	A	999	UC1	OB-C3	2.05	1.41	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	UC1	OB-C3-C4	2.83	119.76	116.39
3	A	999	UC1	C3-C4-CL	2.58	122.39	119.44
3	A	999	UC1	S-C-N	-2.51	118.62	125.29
3	A	999	UC1	C2-C1-N	2.29	127.56	120.13

There are no chirality outliers.

All (3) torsion outliers are listed below:

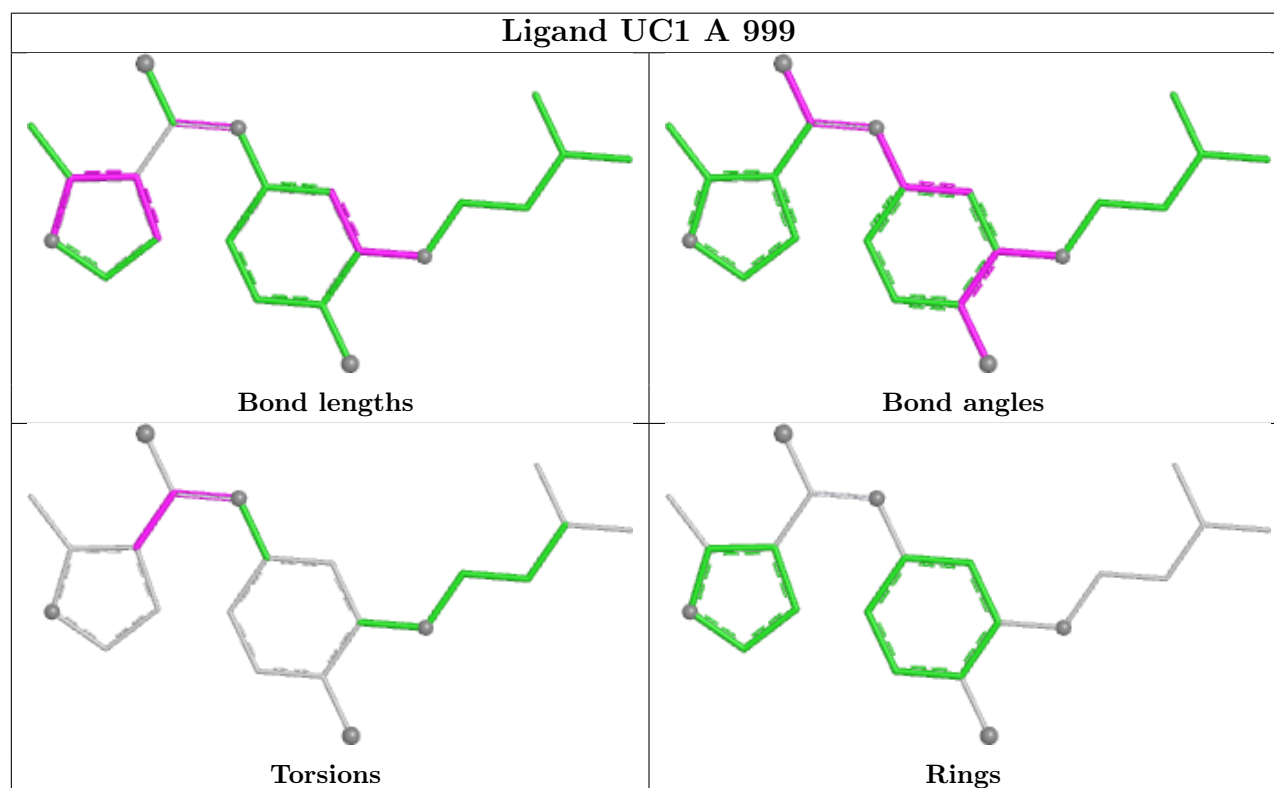
Mol	Chain	Res	Type	Atoms
3	A	999	UC1	C9-C-N-C1
3	A	999	UC1	S-C-N-C1
3	A	999	UC1	N-C-C9-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	UC1	1	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	524/560 (93%)	-0.36	1 (0%) 91 90	38, 70, 122, 150	0
2	B	404/440 (91%)	-0.40	0 100 100	33, 69, 129, 150	0
All	All	928/1000 (92%)	-0.38	1 (0%) 92 91	33, 70, 125, 150	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	PHE	2.6

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	0.96	0.06	50,65,85,86	0

6.3 Carbohydrates [i](#)

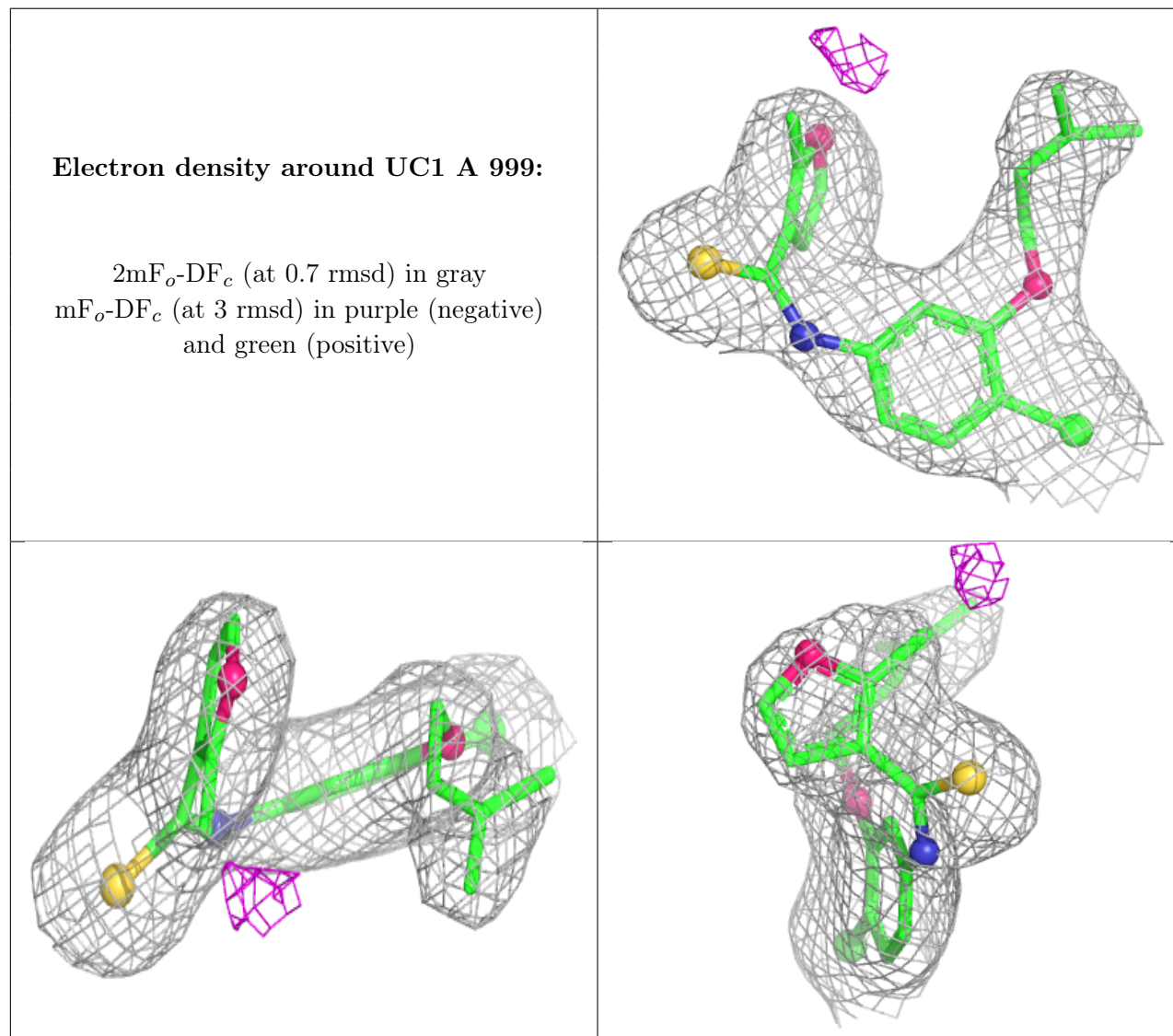
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	UC1	A	999	22/22	0.97	0.07	42,54,62,74	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 ⓘ

There are no such residues in this entry.