



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:31 am BST

PDB ID : 1RT6
Title : HIV-1 REVERSE TRANSCRIPTASE COMPLEXED WITH UC38
Authors : Ren, J.; Stammers, D.K.; Stuart, D.I.
Deposited on : 1998-07-29
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

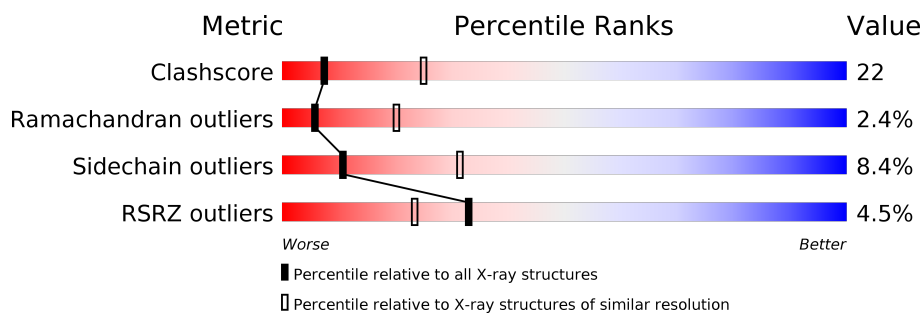
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>4%</div> <div>51%</div> <div>40%</div> <div>5%</div> <div>•</div> </div>
2	B	440	<div> <div>5%</div> <div>56%</div> <div>33%</div> <div>5%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UC3	A	999	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7947 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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4410	2853	734	815	8			

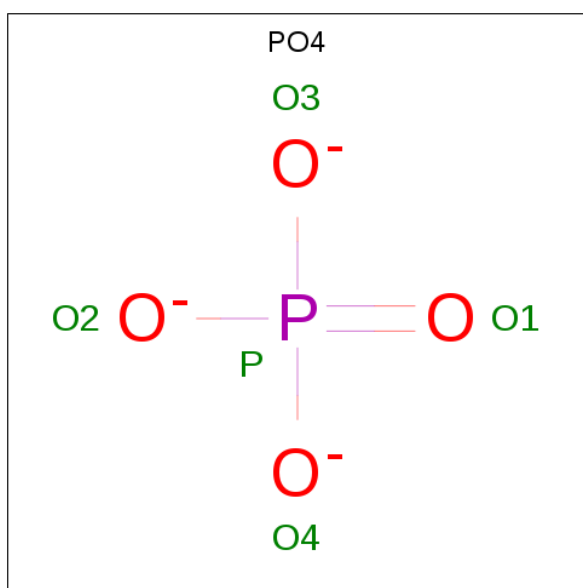
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

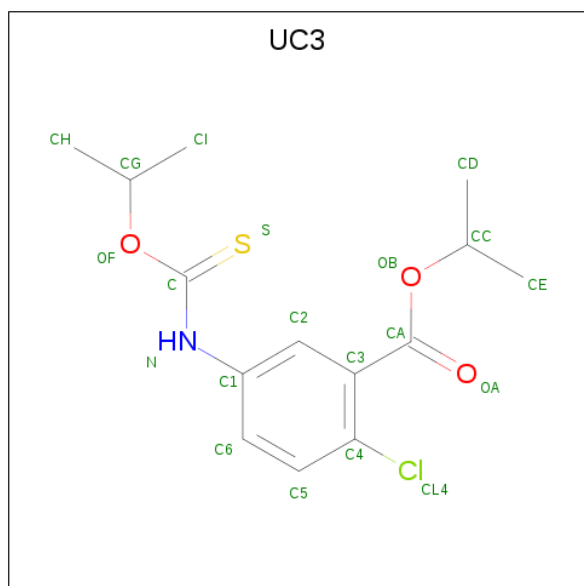
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	0	0
			3416	2221	567	621	7			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1-METHYL ETHYL 2-CHLORO-5-[[[(1-METHYLETHOXY)THIOOXO]METHYL]AMINO]-BENZOATE (three-letter code: UC3) (formula: C₁₄H₁₈ClNO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	
			20	14	1	1	3	1	0

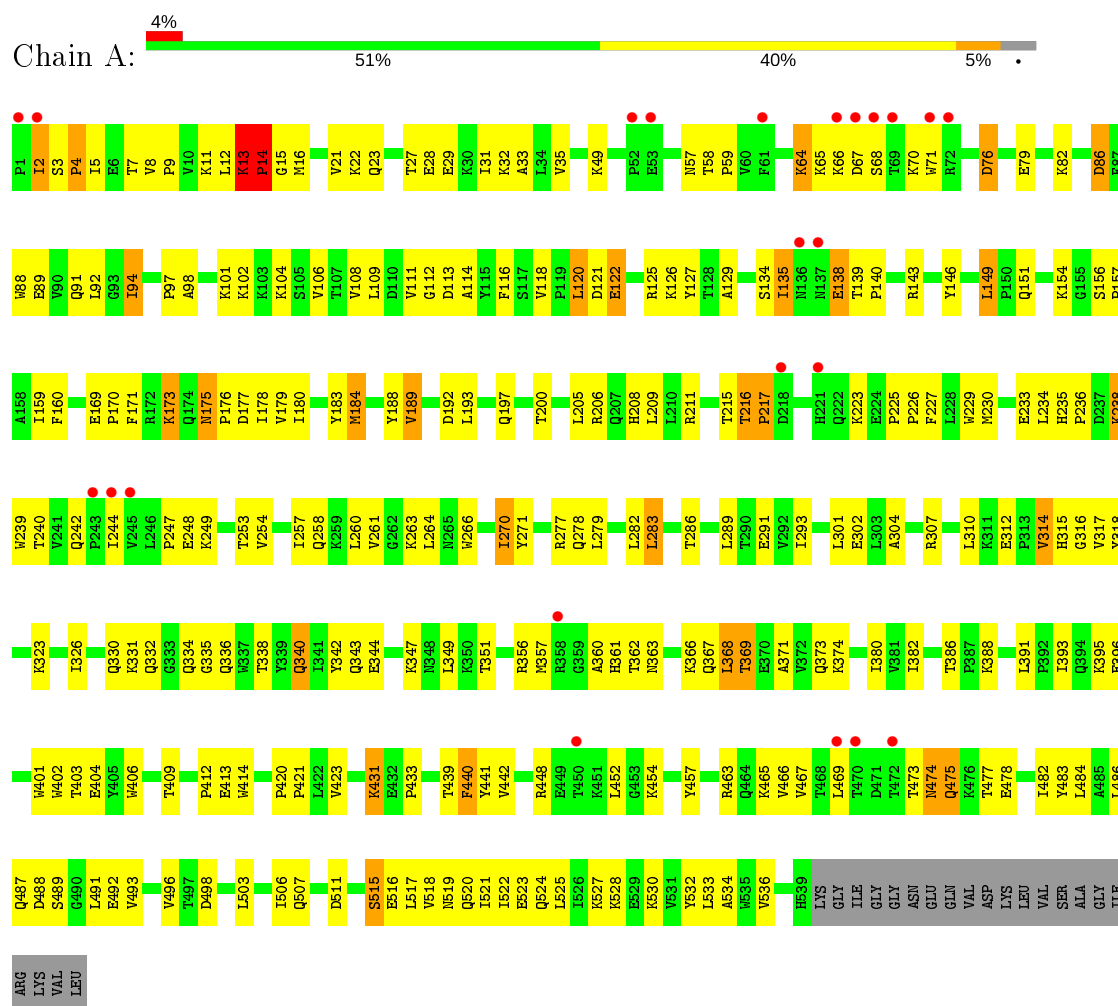
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O	0	0
			54	54		
5	B	42	Total	O	0	0
			42	42		

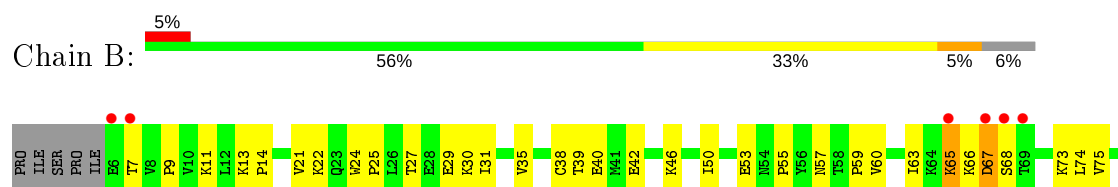
3 Residue-property plots

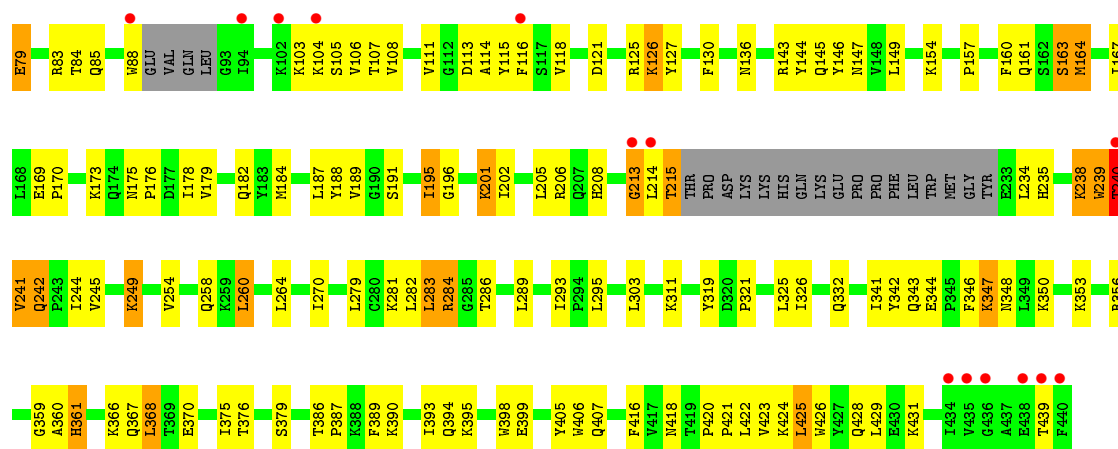
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: HIV-1 REVERSE TRANSCRIPTASE



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.00 Å 109.30 Å 71.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-2.80) 95.8 (29.75-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.80 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.236 , 0.335 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 86.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7947	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, PO4, UC3

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	0.42	0/4519	0.71	4/6143 (0.1%)
2	B	0.43	0/3511	0.68	2/4768 (0.0%)
All	All	0.42	0/8030	0.70	6/10911 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	LYS	C-N-CD	-9.38	99.95	120.60
1	A	13	LYS	C-N-CA	6.80	150.57	122.00
1	A	14	PRO	N-CA-C	6.63	129.35	112.10
2	B	240	THR	N-CA-C	5.44	125.69	111.00
1	A	13	LYS	N-CA-C	5.44	125.69	111.00
2	B	390	LYS	N-CA-C	-5.43	96.33	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4410	0	4453	198	0
2	B	3416	0	3446	158	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	18	7	0
5	A	54	0	0	5	0
5	B	42	0	0	8	0
All	All	7947	0	7917	350	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 22.

All (350) 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:216:THR:HG23	1:A:217:PRO:HD2	1.38	1.03
2:B:241:VAL:HG12	2:B:242:GLN:H	1.28	0.97
2:B:238:LYS:HZ3	2:B:239:TRP:HD1	1.03	0.93
2:B:240:THR:HG23	2:B:350:LYS:HG3	1.51	0.92
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.51	0.91
2:B:240:THR:HB	5:B:1049:HOH:O	1.70	0.91
1:A:188:TYR:CD2	4:A:999:UC3:HE2	2.09	0.86
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.57	0.86
4:A:999:UC3:HI2	4:A:999:UC3:S	2.17	0.85
1:A:216:THR:HG23	1:A:217:PRO:CD	2.07	0.83
1:A:244:ILE:HD11	1:A:263:LYS:HB3	1.60	0.83
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.15	0.82
2:B:113:ASP:HB2	2:B:214:LEU:HD23	1.64	0.79
2:B:240:THR:HG23	2:B:350:LYS:CG	2.15	0.77
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.67	0.77
1:A:326:ILE:HG12	1:A:388:LYS:HE2	1.66	0.77
2:B:118:VAL:HB	2:B:149:LEU:HG	1.67	0.77
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.20	0.76
2:B:84:THR:HB	2:B:154:LYS:HE2	1.69	0.75
1:A:94:ILE:H	1:A:94:ILE:HD13	1.51	0.74
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.18	0.74
2:B:279:LEU:HA	2:B:282:LEU:HD12	1.68	0.73
1:A:9:PRO:HG2	2:B:53:GLU:HG3	1.70	0.73
1:A:371:ALA:HA	1:A:374:LYS:HE3	1.72	0.72
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.70	0.71
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.25	0.71
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.25	0.71
2:B:163:SER:O	2:B:167:ILE:HG23	1.90	0.71
1:A:229:TRP:HB3	1:A:234:LEU:HD21	1.71	0.71
1:A:448:ARG:NE	1:A:474:ASN:H	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.54	0.70
2:B:114:ALA:H	2:B:214:LEU:HD21	1.58	0.69
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.75	0.68
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.76	0.68
1:A:302:GLU:HA	5:A:1020:HOH:O	1.93	0.68
1:A:335:GLY:HA3	1:A:356:ARG:HD2	1.74	0.67
1:A:178:ILE:HD11	1:A:193:LEU:HD11	1.76	0.67
1:A:238:LYS:HB2	1:A:316:GLY:O	1.94	0.67
1:A:448:ARG:HE	1:A:474:ASN:H	1.41	0.67
2:B:29:GLU:HG2	2:B:30:LYS:N	2.10	0.67
1:A:65:LYS:HG2	1:A:66:LYS:H	1.60	0.66
1:A:448:ARG:HH21	1:A:475:GLN:H	1.44	0.66
2:B:241:VAL:CG1	2:B:242:GLN:H	2.04	0.66
1:A:217:PRO:HG2	5:A:1008:HOH:O	1.95	0.65
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.78	0.65
1:A:522:ILE:HA	1:A:525:LEU:HD12	1.78	0.65
2:B:46:LYS:HE2	2:B:116:PHE:CD2	2.31	0.65
2:B:74:LEU:HD12	2:B:75:VAL:H	1.62	0.64
1:A:332:GLN:O	1:A:336:GLN:HB2	1.97	0.64
2:B:27:THR:OG1	2:B:30:LYS:HD3	1.96	0.64
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.79	0.63
2:B:426:TRP:O	2:B:429:LEU:HB2	1.98	0.63
2:B:238:LYS:HG3	2:B:239:TRP:CD1	2.34	0.63
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.79	0.63
1:A:257:ILE:O	1:A:261:VAL:HG23	1.98	0.63
1:A:149:LEU:HD21	1:A:159:ILE:HG22	1.80	0.62
1:A:177:ASP:HB3	5:A:1018:HOH:O	1.98	0.62
2:B:379:SER:CB	2:B:387:PRO:HD3	2.29	0.62
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.82	0.62
1:A:448:ARG:NH2	1:A:475:GLN:H	1.98	0.62
1:A:534:ALA:HB1	5:B:1038:HOH:O	1.99	0.62
2:B:13:LYS:HE3	2:B:84:THR:O	2.00	0.62
2:B:344:GLU:HB3	2:B:347:LYS:HD3	1.83	0.61
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.83	0.61
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.83	0.61
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.36	0.61
1:A:108:VAL:HG11	1:A:223:LYS:HB2	1.82	0.61
2:B:344:GLU:CB	2:B:347:LYS:HD3	2.31	0.61
1:A:122:GLU:CD	1:A:122:GLU:H	2.06	0.59
1:A:135:ILE:O	1:A:138:GLU:HG3	2.03	0.59
2:B:240:THR:HA	2:B:350:LYS:NZ	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.38	0.59
2:B:235:HIS:HB2	2:B:238:LYS:HG2	1.85	0.59
4:A:999:UC3:CI	4:A:999:UC3:S	2.90	0.58
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.85	0.58
1:A:188:TYR:CE2	4:A:999:UC3:HE2	2.39	0.58
1:A:28:GLU:HG3	1:A:29:GLU:N	2.18	0.58
2:B:25:PRO:HD3	5:B:1087:HOH:O	2.03	0.58
1:A:463:ARG:NH1	1:A:488:ASP:O	2.37	0.58
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.39	0.58
1:A:116:PHE:HE1	1:A:151:GLN:HG2	1.67	0.58
2:B:39:THR:O	2:B:42:GLU:HB3	2.03	0.58
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.33	0.57
1:A:234:LEU:HB3	1:A:318:TYR:OH	2.04	0.57
1:A:229:TRP:CB	1:A:234:LEU:HD21	2.34	0.57
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.39	0.57
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.86	0.57
1:A:516:GLU:O	1:A:520:GLN:HG3	2.05	0.57
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.86	0.57
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.87	0.57
1:A:401:TRP:HZ3	1:A:409:THR:HG21	1.69	0.56
2:B:393:ILE:O	2:B:416:PHE:HB3	2.05	0.56
1:A:340:GLN:CB	1:A:351:THR:HG22	2.35	0.56
1:A:515:SER:OG	1:A:518:VAL:HG23	2.05	0.56
1:A:260:LEU:HG	1:A:264:LEU:CD2	2.35	0.56
1:A:31:ILE:O	1:A:35:VAL:HG23	2.06	0.56
1:A:536:VAL:HG12	2:B:258:GLN:HB3	1.87	0.56
2:B:376:THR:CG2	2:B:386:THR:HG22	2.36	0.56
1:A:448:ARG:CZ	1:A:473:THR:HB	2.36	0.56
2:B:421:PRO:O	2:B:425:LEU:HD22	2.06	0.56
1:A:8:VAL:O	1:A:121:ASP:HB2	2.05	0.56
2:B:111:VAL:HA	2:B:214:LEU:HD22	1.86	0.55
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.41	0.55
1:A:254:VAL:HB	1:A:289:LEU:HA	1.87	0.55
1:A:179:VAL:HG11	4:A:999:UC3:HI3	1.87	0.55
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.06	0.55
1:A:492:GLU:HA	1:A:530:LYS:O	2.06	0.55
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.89	0.55
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.21	0.55
1:A:270:ILE:HG21	1:A:314:VAL:HG21	1.88	0.54
1:A:323:LYS:NZ	1:A:344:GLU:HG3	2.21	0.54
1:A:331:LYS:CE	1:A:334:GLN:HA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:THR:HG22	5:B:1050:HOH:O	2.07	0.54
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.90	0.54
1:A:64:LYS:H	1:A:64:LYS:HD2	1.73	0.54
2:B:11:LYS:HB2	2:B:85:GLN:OE1	2.07	0.54
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.88	0.54
1:A:205:LEU:O	1:A:209:LEU:HG	2.08	0.54
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.90	0.54
1:A:247:PRO:C	1:A:307:ARG:HH22	2.10	0.53
1:A:516:GLU:O	1:A:519:ASN:HB2	2.08	0.53
2:B:213:GLY:O	2:B:214:LEU:HG	2.08	0.53
1:A:13:LYS:HG2	1:A:16:MET:SD	2.47	0.53
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.90	0.53
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.09	0.53
1:A:58:THR:HG23	1:A:76:ASP:O	2.08	0.53
2:B:395:LYS:O	2:B:399:GLU:HG3	2.08	0.53
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.43	0.53
2:B:245:VAL:HG13	2:B:431:LYS:HB2	1.90	0.53
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.91	0.53
2:B:125:ARG:NE	2:B:147:ASN:HA	2.24	0.53
2:B:240:THR:HA	2:B:350:LYS:HZ2	1.73	0.53
1:A:271:TYR:HE1	1:A:312:GLU:O	1.92	0.53
1:A:129:ALA:HB1	1:A:143:ARG:NH1	2.21	0.52
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.44	0.52
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.39	0.52
1:A:65:LYS:HG2	1:A:66:LYS:N	2.24	0.52
1:A:227:PHE:HD2	4:A:999:UC3:CL4	2.29	0.52
2:B:107:THR:O	2:B:188:TYR:HA	2.09	0.52
2:B:169:GLU:O	2:B:173:LYS:HD3	2.10	0.52
2:B:29:GLU:HG2	2:B:30:LYS:H	1.74	0.52
2:B:422:LEU:HB2	5:B:1093:HOH:O	2.10	0.52
1:A:518:VAL:O	1:A:522:ILE:HG13	2.09	0.52
2:B:244:ILE:HG21	2:B:426:TRP:CZ2	2.45	0.52
1:A:483:TYR:CE1	1:A:524:GLN:HG3	2.44	0.51
2:B:281:LYS:O	2:B:284:ARG:HB3	2.09	0.51
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.10	0.51
1:A:439:THR:HG23	2:B:289:LEU:HD13	1.93	0.51
1:A:135:ILE:H	1:A:135:ILE:HD12	1.75	0.51
1:A:234:LEU:HD12	1:A:239:TRP:HB3	1.92	0.51
1:A:371:ALA:CA	1:A:374:LYS:HE3	2.40	0.51
2:B:234:LEU:HD12	2:B:234:LEU:N	2.26	0.51
1:A:283:LEU:O	1:A:286:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:CE2	1:A:146:TYR:HE2	2.29	0.50
1:A:139:THR:HB	1:A:140:PRO:CD	2.42	0.50
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.93	0.50
2:B:356:ARG:HH12	2:B:359:GLY:H	1.60	0.50
2:B:238:LYS:HG3	2:B:239:TRP:HD1	1.75	0.50
2:B:356:ARG:NH2	2:B:361:HIS:HB3	2.26	0.50
1:A:116:PHE:HE1	1:A:151:GLN:CG	2.25	0.50
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.94	0.50
1:A:473:THR:OG1	1:A:475:GLN:HG3	2.11	0.50
2:B:205:LEU:O	2:B:208:HIS:HB3	2.12	0.49
1:A:88:TRP:HE3	1:A:88:TRP:HA	1.77	0.49
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.93	0.49
2:B:114:ALA:N	2:B:214:LEU:HD21	2.24	0.49
1:A:13:LYS:HB3	1:A:14:PRO:O	2.12	0.49
1:A:206:ARG:NE	1:A:216:THR:CG2	2.76	0.49
1:A:278:GLN:O	1:A:282:LEU:HD13	2.12	0.49
2:B:208:HIS:HB2	5:B:1045:HOH:O	2.12	0.49
1:A:206:ARG:HE	1:A:216:THR:CG2	2.25	0.49
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.27	0.49
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.95	0.49
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.95	0.49
1:A:483:TYR:HE1	1:A:524:GLN:HG3	1.78	0.49
1:A:431:LYS:HE3	1:A:431:LYS:HA	1.95	0.49
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.95	0.49
1:A:366:LYS:O	1:A:369:THR:HB	2.13	0.48
2:B:202:ILE:O	2:B:205:LEU:HB3	2.13	0.48
1:A:483:TYR:HE1	1:A:524:GLN:CG	2.26	0.48
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.49	0.48
1:A:360:ALA:HB1	1:A:361:HIS:HD2	1.78	0.48
2:B:126:LYS:HG2	2:B:127:TYR:N	2.28	0.48
1:A:68:SER:C	1:A:70:LYS:H	2.15	0.48
2:B:368:LEU:HD13	2:B:398:TRP:CZ3	2.49	0.48
2:B:113:ASP:O	2:B:116:PHE:HD1	1.97	0.48
1:A:135:ILE:N	1:A:135:ILE:HD12	2.29	0.47
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.96	0.47
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.96	0.47
1:A:14:PRO:O	1:A:16:MET:N	2.46	0.47
1:A:171:PHE:O	1:A:175:ASN:ND2	2.47	0.47
2:B:106:VAL:HA	2:B:189:VAL:O	2.14	0.47
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.29	0.47
2:B:242:GLN:HA	2:B:242:GLN:NE2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TYR:CD1	1:A:184:MET:HB2	2.50	0.47
1:A:206:ARG:NE	1:A:216:THR:HG21	2.30	0.47
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.97	0.47
1:A:116:PHE:CE1	1:A:151:GLN:HG2	2.49	0.47
1:A:486:LEU:O	1:A:528:LYS:NZ	2.48	0.47
2:B:167:ILE:O	2:B:208:HIS:CE1	2.68	0.47
1:A:109:LEU:HD21	1:A:206:ARG:HG2	1.97	0.47
1:A:420:PRO:HA	1:A:421:PRO:C	2.35	0.47
1:A:253:THR:O	1:A:257:ILE:HG13	2.15	0.46
2:B:260:LEU:O	2:B:264:LEU:HG	2.14	0.46
2:B:356:ARG:CZ	2:B:361:HIS:HB3	2.44	0.46
1:A:106:VAL:HG23	1:A:236:PRO:HB3	1.98	0.46
1:A:466:VAL:HG12	1:A:467:VAL:N	2.30	0.46
2:B:173:LYS:O	2:B:176:PRO:HD3	2.16	0.46
2:B:178:ILE:HG12	2:B:191:SER:CB	2.45	0.46
2:B:31:ILE:O	2:B:35:VAL:HG23	2.15	0.46
2:B:240:THR:H	2:B:350:LYS:HZ3	1.64	0.46
1:A:134:SER:HB3	1:A:138:GLU:H	1.80	0.46
1:A:27:THR:O	1:A:31:ILE:HG13	2.16	0.46
2:B:27:THR:O	2:B:31:ILE:HG13	2.15	0.46
2:B:326:ILE:O	2:B:341:ILE:HA	2.16	0.46
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.96	0.46
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.51	0.46
1:A:484:LEU:HD23	1:A:487:GLN:OE1	2.14	0.46
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.98	0.46
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.97	0.46
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.98	0.46
1:A:248:GLU:HB2	1:A:307:ARG:HH21	1.81	0.46
1:A:126:LYS:HE2	1:A:127:TYR:CZ	2.51	0.45
2:B:114:ALA:HB2	2:B:214:LEU:HD11	1.97	0.45
2:B:29:GLU:CG	2:B:30:LYS:N	2.79	0.45
1:A:79:GLU:O	1:A:82:LYS:HG2	2.16	0.45
1:A:293:ILE:HD12	1:A:293:ILE:N	2.31	0.45
2:B:332:GLN:NE2	2:B:428:GLN:HB2	2.31	0.45
1:A:240:THR:HG22	1:A:315:HIS:CG	2.52	0.45
1:A:440:PHE:CD1	1:A:440:PHE:N	2.85	0.45
1:A:28:GLU:HG3	1:A:29:GLU:H	1.80	0.45
1:A:441:TYR:CD1	2:B:286:THR:HG23	2.52	0.45
1:A:68:SER:C	1:A:70:LYS:N	2.69	0.45
2:B:160:PHE:O	2:B:164:MET:HB2	2.16	0.45
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HG23	2:B:196:GLY:H	1.82	0.45
2:B:249:LYS:HB2	2:B:249:LYS:HE2	1.84	0.45
2:B:178:ILE:HG23	2:B:191:SER:HB3	1.99	0.45
2:B:240:THR:CA	2:B:350:LYS:NZ	2.80	0.45
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.99	0.45
2:B:325:LEU:HA	2:B:343:GLN:HG2	1.98	0.45
2:B:393:ILE:HG12	2:B:394:GLN:N	2.32	0.45
1:A:301:LEU:O	1:A:304:ALA:HB3	2.18	0.44
2:B:65:LYS:O	2:B:67:ASP:N	2.50	0.44
2:B:130:PHE:CE1	2:B:144:TYR:HD2	2.35	0.44
2:B:241:VAL:CG1	2:B:242:GLN:N	2.78	0.44
1:A:151:GLN:HG3	5:A:1074:HOH:O	2.17	0.44
2:B:195:ILE:HG23	2:B:196:GLY:N	2.32	0.44
2:B:240:THR:HG23	2:B:350:LYS:CD	2.47	0.44
2:B:104:LYS:O	2:B:235:HIS:HA	2.17	0.44
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.98	0.44
1:A:517:LEU:O	1:A:521:ILE:HG13	2.18	0.44
2:B:353:LYS:HB2	2:B:353:LYS:HE3	1.86	0.44
1:A:139:THR:HB	1:A:140:PRO:HD2	1.99	0.44
2:B:106:VAL:HB	2:B:234:LEU:HB2	2.00	0.44
2:B:241:VAL:HG12	2:B:242:GLN:N	2.12	0.44
2:B:244:ILE:HG23	2:B:429:LEU:HB3	1.99	0.44
1:A:101:LYS:O	4:A:999:UC3:N	2.46	0.43
1:A:489:SER:HB2	1:A:493:VAL:HG22	2.00	0.43
2:B:239:TRP:HB2	2:B:240:THR:H	1.42	0.43
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.16	0.43
1:A:122:GLU:CD	1:A:122:GLU:N	2.71	0.43
1:A:277:ARG:HD2	5:A:1077:HOH:O	2.16	0.43
1:A:253:THR:HA	1:A:291:GLU:O	2.17	0.43
1:A:395:LYS:HG2	1:A:414:TRP:CZ2	2.53	0.43
2:B:79:GLU:HG3	2:B:83:ARG:HH21	1.83	0.43
2:B:283:LEU:HD12	2:B:283:LEU:HA	1.86	0.43
1:A:101:LYS:N	1:A:101:LYS:HD2	2.33	0.43
1:A:206:ARG:HE	1:A:216:THR:HG21	1.82	0.43
1:A:205:LEU:O	1:A:208:HIS:HB3	2.19	0.43
1:A:454:LYS:HA	1:A:467:VAL:O	2.19	0.43
1:A:368:LEU:HD21	1:A:391:LEU:HD22	2.01	0.43
1:A:94:ILE:H	1:A:94:ILE:CD1	2.27	0.43
1:A:122:GLU:HA	1:A:125:ARG:CD	2.49	0.43
1:A:448:ARG:HH21	1:A:475:GLN:N	2.12	0.43
2:B:205:LEU:HD13	2:B:205:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.54	0.43
1:A:197:GLN:O	1:A:200:THR:HB	2.18	0.42
2:B:24:TRP:HB2	2:B:25:PRO:HD2	2.01	0.42
1:A:169:GLU:O	1:A:173:LYS:HD3	2.19	0.42
2:B:105:SER:HA	2:B:234:LEU:O	2.19	0.42
2:B:53:GLU:O	2:B:55:PRO:HD3	2.19	0.42
1:A:57:ASN:HA	1:A:129:ALA:O	2.19	0.42
1:A:2:ILE:HG22	1:A:3:SER:H	1.84	0.42
2:B:157:PRO:HG3	2:B:184:MET:HA	2.00	0.42
2:B:108:VAL:HG22	2:B:188:TYR:HD2	1.84	0.42
1:A:216:THR:HG23	1:A:217:PRO:N	2.34	0.42
1:A:233:GLU:HG3	1:A:242:GLN:HG2	2.01	0.42
1:A:235:HIS:O	1:A:318:TYR:HE2	2.03	0.42
1:A:506:ILE:HG12	1:A:533:LEU:HB3	2.01	0.42
2:B:420:PRO:HB2	2:B:423:VAL:HG23	2.01	0.42
1:A:382:ILE:O	2:B:136:ASN:HB2	2.19	0.42
2:B:160:PHE:CD2	2:B:160:PHE:O	2.73	0.42
2:B:173:LYS:N	2:B:173:LYS:HD2	2.34	0.42
2:B:164:MET:HG2	2:B:182:GLN:NE2	2.35	0.42
2:B:366:LYS:O	2:B:370:GLU:HG3	2.19	0.42
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.90	0.42
1:A:533:LEU:HA	1:A:533:LEU:HD12	1.63	0.42
2:B:125:ARG:HE	2:B:147:ASN:HA	1.83	0.42
2:B:254:VAL:O	2:B:258:GLN:HG3	2.19	0.42
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.55	0.42
2:B:73:LYS:HE2	2:B:146:TYR:OH	2.20	0.42
1:A:478:GLU:O	1:A:482:ILE:HG13	2.20	0.41
1:A:498:ASP:HA	1:A:536:VAL:O	2.20	0.41
1:A:64:LYS:HE3	1:A:71:TRP:CZ3	2.55	0.41
1:A:33:ALA:HB1	1:A:71:TRP:HB3	2.02	0.41
2:B:63:ILE:HD13	2:B:74:LEU:CD2	2.48	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.19	0.41
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.48	0.41
2:B:254:VAL:HG22	2:B:293:ILE:HD11	2.02	0.41
2:B:88:TRP:N	2:B:88:TRP:CD1	2.88	0.41
1:A:260:LEU:C	1:A:264:LEU:HD23	2.41	0.41
2:B:35:VAL:O	2:B:39:THR:HG23	2.20	0.41
1:A:254:VAL:O	1:A:258:GLN:HG3	2.19	0.41
1:A:395:LYS:HG2	1:A:414:TRP:CH2	2.55	0.41
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.85	0.41
1:A:371:ALA:HA	1:A:374:LYS:CE	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:HG21	1:A:120:LEU:O	2.21	0.41
2:B:295:LEU:HD23	2:B:295:LEU:HA	1.91	0.41
1:A:175:ASN:HA	1:A:176:PRO:HD2	1.89	0.41
2:B:108:VAL:HA	2:B:187:LEU:O	2.20	0.41
2:B:206:ARG:HD2	2:B:215:THR:HB	2.02	0.41
2:B:279:LEU:O	2:B:282:LEU:N	2.53	0.41
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.92	0.41
1:A:266:TRP:C	1:A:266:TRP:CD1	2.94	0.41
1:A:475:GLN:HA	1:A:478:GLU:OE1	2.21	0.41
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.56	0.41
1:A:279:LEU:HD23	1:A:302:GLU:OE2	2.20	0.41
1:A:523:GLU:O	1:A:527:LYS:HG3	2.21	0.41
2:B:74:LEU:HD12	2:B:75:VAL:N	2.32	0.41
1:A:116:PHE:CE2	1:A:146:TYR:CE2	3.09	0.41
2:B:111:VAL:O	2:B:111:VAL:HG23	2.21	0.41
2:B:240:THR:CG2	5:B:1050:HOH:O	2.67	0.41
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.56	0.41
1:A:519:ASN:HA	1:A:522:ILE:HD12	2.03	0.40
2:B:106:VAL:HG12	2:B:107:THR:N	2.36	0.40
2:B:161:GLN:HE22	2:B:182:GLN:NE2	2.19	0.40
2:B:235:HIS:O	2:B:238:LYS:HG2	2.21	0.40
2:B:35:VAL:HA	5:B:1040:HOH:O	2.21	0.40
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.56	0.40
1:A:395:LYS:NZ	1:A:414:TRP:CE2	2.81	0.40
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.56	0.40
2:B:240:THR:CA	2:B:350:LYS:HZ3	2.34	0.40
2:B:406:TRP:O	2:B:407:GLN:HG3	2.22	0.40
2:B:7:THR:HB	2:B:121:ASP:HA	2.04	0.40
1:A:406:TRP:HB3	1:A:507:GLN:HG2	2.02	0.40
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.20	0.40
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.56	0.40
1:A:86:ASP:HA	1:A:154:LYS:HZ1	1.86	0.40
2:B:238:LYS:NZ	2:B:239:TRP:CD1	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	536/560 (96%)	475 (89%)	46 (9%)	15 (3%)	5	17
2	B	408/440 (93%)	364 (89%)	36 (9%)	8 (2%)	7	24
All	All	944/1000 (94%)	839 (89%)	82 (9%)	23 (2%)	6	20

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	14	PRO
1	A	15	GLY
1	A	112	GLY
1	A	217	PRO
1	A	230	MET
2	B	66	LYS
2	B	241	VAL
1	A	91	GLN
1	A	122	GLU
1	A	412	PRO
2	B	195	ILE
2	B	240	THR
1	A	4	PRO
2	B	68	SER
2	B	213	GLY
2	B	242	GLN
1	A	67	ASP
1	A	2	ILE
1	A	138	GLU
1	A	135	ILE
2	B	14	PRO
1	A	270	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	483/499 (97%)	435 (90%)	48 (10%)	8	23
2	B	375/400 (94%)	351 (94%)	24 (6%)	17	45
All	All	858/899 (95%)	786 (92%)	72 (8%)	11	31

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	11	LYS
1	A	13	LYS
1	A	22	LYS
1	A	32	LYS
1	A	49	LYS
1	A	64	LYS
1	A	76	ASP
1	A	86	ASP
1	A	89	GLU
1	A	92	LEU
1	A	94	ILE
1	A	97	PRO
1	A	102	LYS
1	A	113	ASP
1	A	120	LEU
1	A	149	LEU
1	A	173	LYS
1	A	175	ASN
1	A	184	MET
1	A	189	VAL
1	A	211	ARG
1	A	215	THR
1	A	216	THR
1	A	238	LYS
1	A	249	LYS
1	A	283	LEU

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Mol	Chain	Res	Type
1	A	314	VAL
1	A	340	GLN
1	A	357	MET
1	A	362	THR
1	A	368	LEU
1	A	369	THR
1	A	373	GLN
1	A	396	GLU
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	413	GLU
1	A	431	LYS
1	A	440	PHE
1	A	452	LEU
1	A	465	LYS
1	A	474	ASN
1	A	475	GLN
1	A	491	LEU
1	A	496	VAL
1	A	515	SER
2	B	22	LYS
2	B	40	GLU
2	B	65	LYS
2	B	67	ASP
2	B	79	GLU
2	B	126	LYS
2	B	163	SER
2	B	164	MET
2	B	201	LYS
2	B	215	THR
2	B	238	LYS
2	B	239	TRP
2	B	240	THR
2	B	249	LYS
2	B	260	LEU
2	B	283	LEU
2	B	284	ARG
2	B	303	LEU
2	B	311	LYS
2	B	347	LYS
2	B	361	HIS

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Mol	Chain	Res	Type
2	B	368	LEU
2	B	425	LEU
2	B	439	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	174	GLN
1	A	278	GLN
1	A	332	GLN
1	A	361	HIS
1	A	407	GLN
1	A	475	GLN
1	A	512	GLN
2	B	57	ASN
2	B	175	ASN
2	B	182	GLN
2	B	197	GLN
2	B	242	GLN
2	B	332	GLN
2	B	334	GLN
2	B	394	GLN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	A	280	1	3,7,8	0.89	0	1,8,10	5.31	1 (100%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	280	CSD	OD1-SG-CB	5.31	115.64	105.54

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	$\# Z > 2$
4	UC3	A	999	-	20,20,20	2.59	5 (25%)	26,27,27	0.90	2 (7%)
3	PO4	A	1000	-	4,4,4	1.77	2 (50%)	6,6,6	0.40	0

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
4	UC3	A	999	-	-	8/16/16/16	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	UC3	C-N	9.25	1.42	1.34
4	A	999	UC3	OF-C	3.66	1.38	1.33
3	A	1000	PO4	P-O4	-2.23	1.47	1.54
4	A	999	UC3	C-S	2.17	1.69	1.66
3	A	1000	PO4	P-O2	-2.13	1.48	1.54
4	A	999	UC3	C1-N	2.03	1.45	1.41
4	A	999	UC3	C3-CA	2.02	1.54	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	UC3	CC-OB-CA	-2.87	113.11	117.48
4	A	999	UC3	OF-C-S	2.60	127.84	125.61

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	UC3	S-C-OF-CG
4	A	999	UC3	N-C-OF-CG
4	A	999	UC3	C3-CA-OB-CC
4	A	999	UC3	CH-CG-OF-C
4	A	999	UC3	CI-CG-OF-C
4	A	999	UC3	OA-CA-OB-CC

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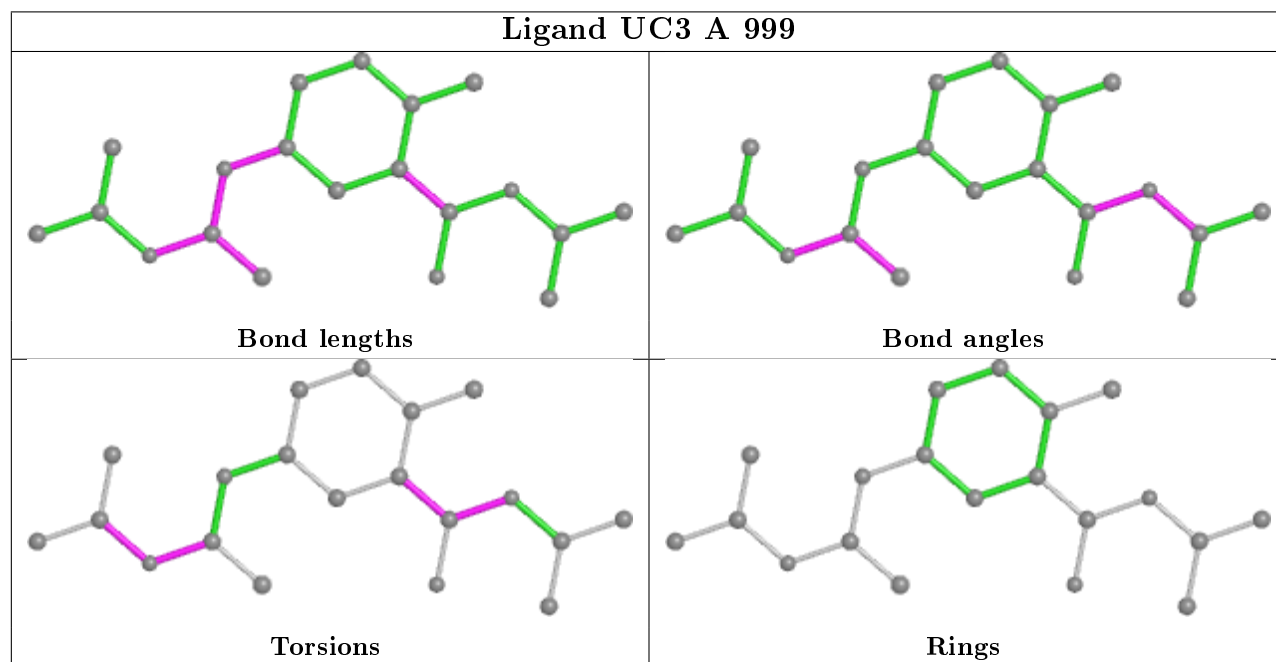
Mol	Chain	Res	Type	Atoms
4	A	999	UC3	C4-C3-CA-OB
4	A	999	UC3	C2-C3-CA-OB

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	UC3	7	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	538/560 (96%)	-0.04	23 (4%)	35	25	10, 55, 113, 164	0
2	B	414/440 (94%)	-0.03	20 (4%)	30	21	11, 51, 113, 156	0
All	All	952/1000 (95%)	-0.04	43 (4%)	33	23	10, 54, 113, 164	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	VAL	6.1
1	A	67	ASP	6.1
2	B	88	TRP	6.0
2	B	435	VAL	5.6
1	A	68	SER	5.3
2	B	69	THR	4.7
1	A	52	PRO	4.5
2	B	438	GLU	4.5
1	A	221	HIS	4.4
2	B	434	ILE	4.2
2	B	67	ASP	3.8
1	A	358	ARG	3.7
2	B	6	GLU	3.5
2	B	436	GLY	3.4
1	A	1	PRO	3.4
2	B	439	THR	3.3
2	B	240	THR	3.3
1	A	66	LYS	3.3
2	B	440	PHE	3.3
1	A	53	GLU	3.2
2	B	7	THR	3.1
1	A	218	ASP	3.0
2	B	213	GLY	2.9
2	B	65	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	2.9
1	A	136	ASN	2.8
1	A	72	ARG	2.8
2	B	116	PHE	2.7
2	B	68	SER	2.7
1	A	469	LEU	2.6
1	A	470	THR	2.6
1	A	2	ILE	2.6
1	A	450	THR	2.6
2	B	94	ILE	2.4
1	A	61	PHE	2.4
1	A	244	ILE	2.2
2	B	102	LYS	2.2
1	A	243	PRO	2.2
1	A	71	TRP	2.1
2	B	214	LEU	2.1
1	A	137	ASN	2.1
1	A	472	THR	2.0
2	B	104	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.95	0.15	35,41,45,55	0

6.3 Carbohydrates ⓘ

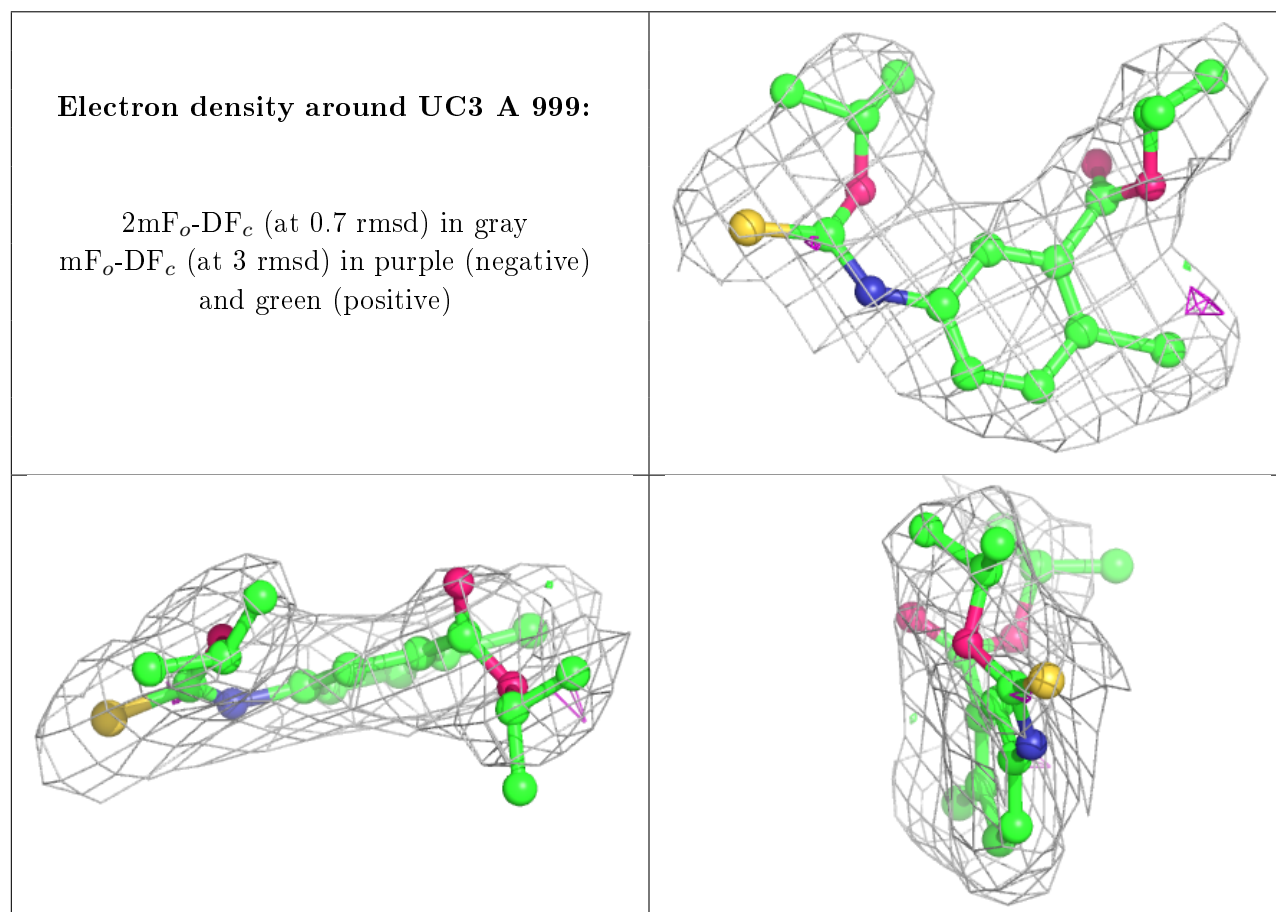
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
3	PO4	A	1000	5/5	0.90	0.22	93,102,109,114	0
4	UC3	A	999	20/20	0.95	0.14	11,30,64,86	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.