Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 11:18 AM EST

PDB ID	:	3QLH
Title	:	HIV-1 Reverse Transcriptase in Complex with Manicol at the RNase H Active Site and TMC278 (Rilpivirine) at the NNRTI Binding Pocket
Authors	:	Himmel, D.M.; Wojtak, K.; Bauman, J.D.; Arnold, E.
Deposited on	:	2011-02-02
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:

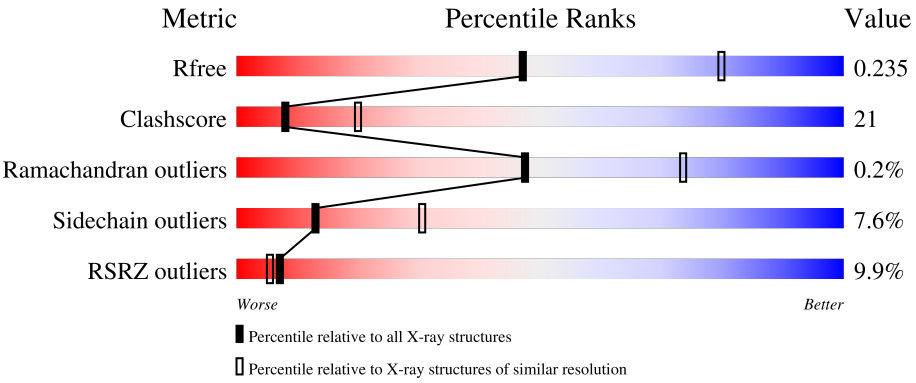
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	555	10% 68% 27% 5%
2	B	423	9% 60% 32% . . .

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8044 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/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	555	4509	2918	749	835	7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

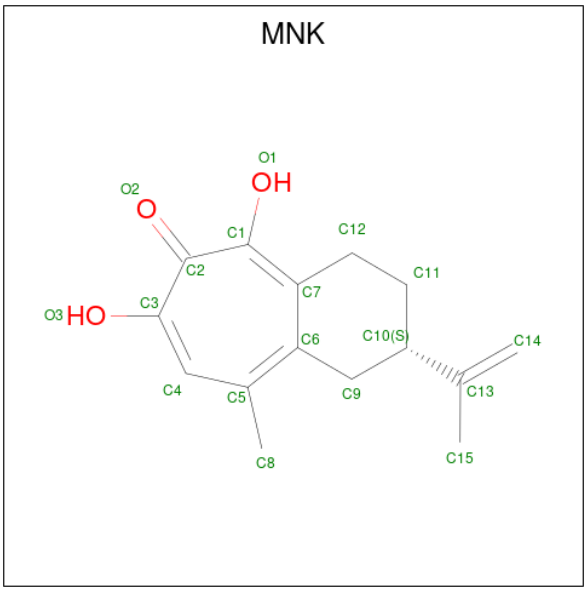
- Molecule 2 is a protein called reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	407	3376	2200	558	611	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

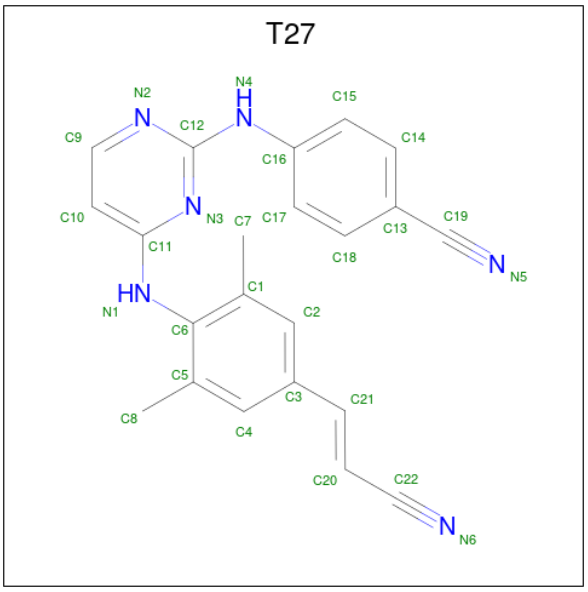
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is (2S)-5,7-dihydroxy-9-methyl-2-(prop-1-en-2-yl)-1,2,3,4-tetrahydro-6H-benzo[7]annulen-6-one (three-letter code: MNK) (formula: $C_{15}H_{18}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 18 15 3	0	0

- Molecule 4 is 4-{[4-({4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl}amino)pyrimidin-2-yl]amino}benzonitrile (three-letter code: T27) (formula: $C_{22}H_{18}N_6$).

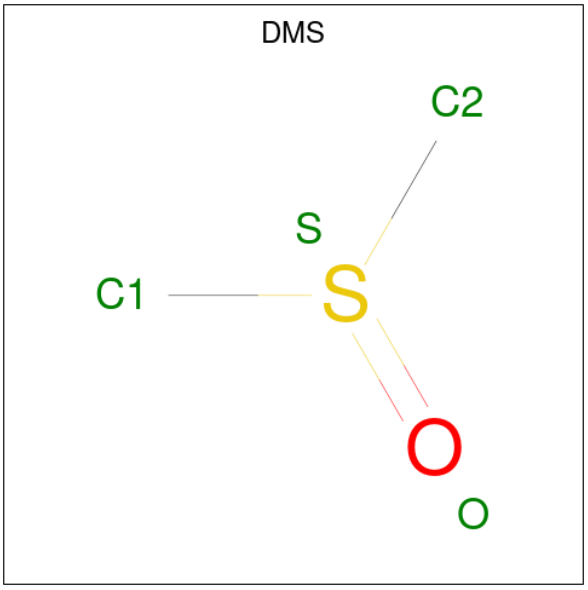


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 28 22 6	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

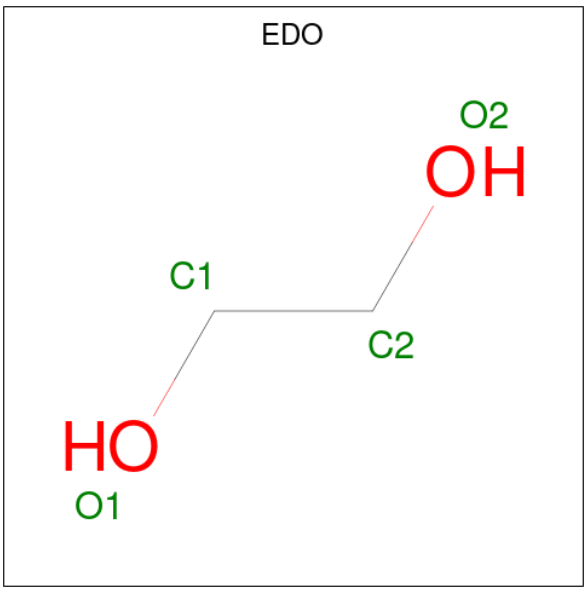
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mn 2 2	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O S 4 2 1 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

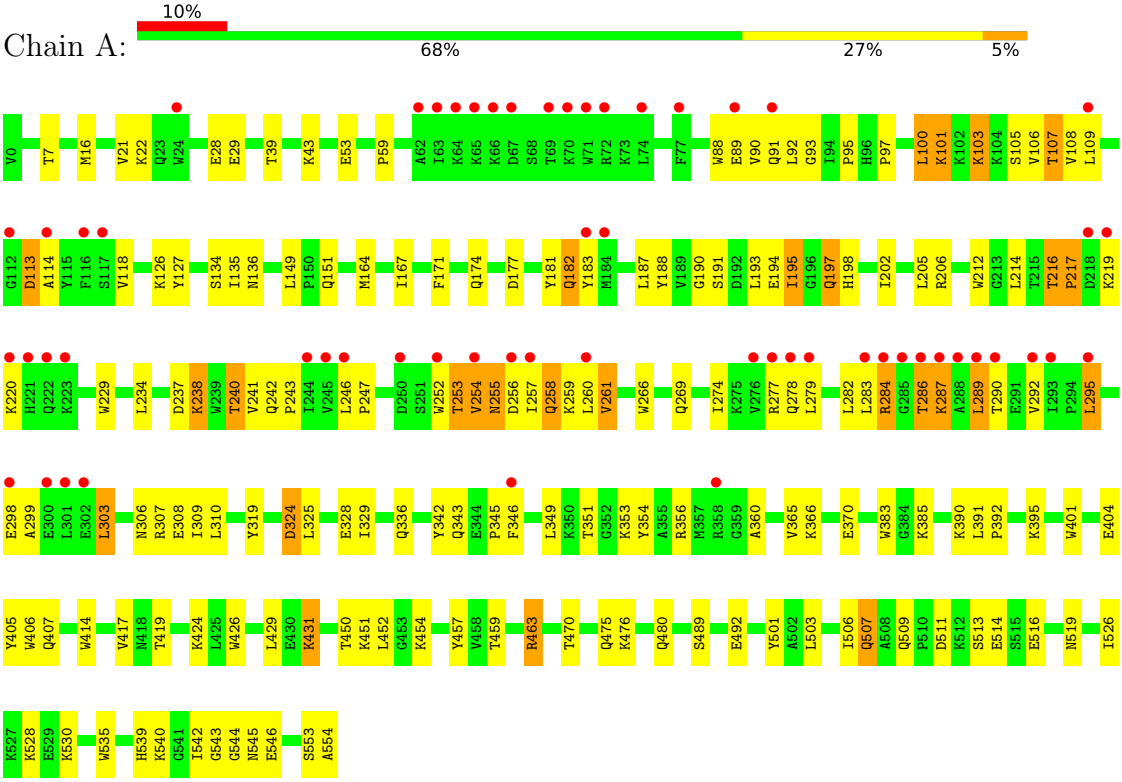
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	52	Total O 52 52	0	0
8	B	51	Total O 51 51	0	0

3 Residue-property plots (i)

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.

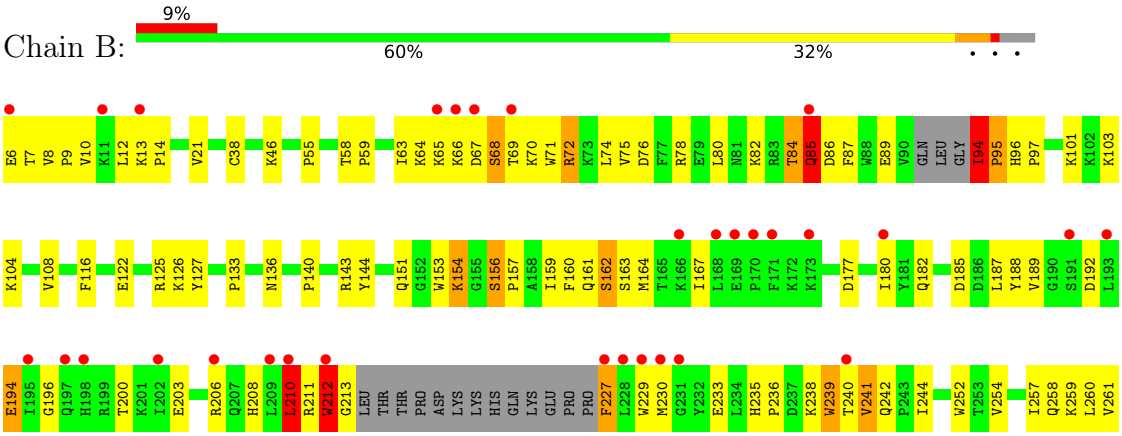
• Molecule 1: reverse transcriptase/ribonuclease H

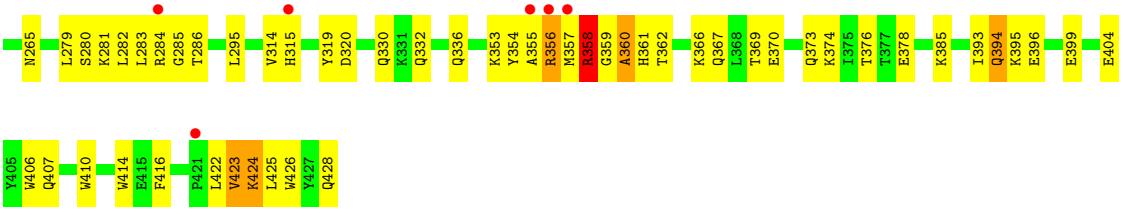
Chain A:



• Molecule 2: reverse transcriptase/ribonuclease H

Chain B:




N265
L279
S280
K281
L282
L283
R284
G285
T286
L295
V314
H315
Y319
D320
Q330
K331
Q332
Q336
K353
Y354
A355
R356
M357
R358
G359
A360
H361
T362
K366
Q367
L368
T369
E370
Q373
K374
I375
T376
T377
E378
K385
I393
Q394
K395
E396
E399
E404
Y405
W406
Q407
W410
W414
E415
F416
P421
L422
V423
K424
L425
W426
Y427
Q428

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.93Å 72.98Å 108.38Å 90.00° 101.11° 90.00°	Depositor
Resolution (Å)	43.21 – 2.70 43.21 – 2.69	Depositor EDS
% Data completeness (in resolution range)	95.8 (43.21-2.70) 94.9 (43.21-2.69)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.251 0.218 , 0.235	Depositor DCC
R_{free} test set	995 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8044	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: DMS, MNK, T27, EDO, MN

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	0.45	0/4627	0.61	0/6289
2	B	0.42	0/3473	0.58	0/4715
All	All	0.43	0/8100	0.60	0/11004

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	B	0	11
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	THR	Peptide
1	A	217	PRO	Peptide
1	A	240	THR	Peptide
1	A	284	ARG	Peptide
1	A	287	LYS	Peptide
2	B	194	GLU	Peptide
2	B	210	LEU	Peptide
2	B	239	TRP	Peptide
2	B	356	ARG	Peptide

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Mol	Chain	Res	Type	Group
2	B	357	MET	Peptide
2	B	358	ARG	Peptide
2	B	360	ALA	Peptide
2	B	85	GLN	Peptide
2	B	89	GLU	Peptide
2	B	94	ILE	Peptide
2	B	95	PRO	Peptide

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	4509	0	4563	186	0
2	B	3376	0	3398	165	0
3	A	18	0	17	5	0
4	A	28	0	18	1	0
5	A	2	0	0	0	0
6	B	4	0	6	3	0
7	B	4	0	6	1	0
8	A	52	0	0	4	0
8	B	51	0	0	1	0
All	All	8044	0	8008	342	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 21.

All (342) 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:239:TRP:CA	2:B:240:THR:HG22	1.62	1.30
2:B:80:LEU:O	2:B:84:THR:HG22	1.42	1.17
1:A:507:GLN:CA	1:A:507:GLN:HE21	1.53	1.16
1:A:242:GLN:HB3	1:A:243:PRO:CD	1.78	1.12
1:A:240:THR:HG23	1:A:241:VAL:O	1.50	1.10
1:A:507:GLN:HA	1:A:507:GLN:NE2	1.64	1.07
1:A:507:GLN:HE21	1:A:507:GLN:HA	0.91	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ILE:HG13	2:B:94:ILE:O	1.44	1.05
1:A:242:GLN:HB3	1:A:243:PRO:HD2	1.06	1.04
2:B:239:TRP:HA	2:B:240:THR:HG22	1.03	1.03
2:B:241:VAL:CG2	2:B:242:GLN:H	1.72	1.03
2:B:239:TRP:HA	2:B:240:THR:CG2	1.88	1.02
2:B:360:ALA:HB2	2:B:367:GLN:HE21	1.26	1.00
2:B:360:ALA:CB	2:B:367:GLN:NE2	2.25	0.99
1:A:92:LEU:HD12	1:A:93:GLY:N	1.78	0.99
2:B:336:GLN:HE21	2:B:355:ALA:CB	1.76	0.97
2:B:360:ALA:HB1	2:B:361:HIS:HA	1.45	0.97
2:B:360:ALA:HB1	2:B:361:HIS:CA	1.95	0.96
2:B:241:VAL:HG22	2:B:242:GLN:N	1.79	0.95
2:B:241:VAL:HG22	2:B:242:GLN:H	1.34	0.92
2:B:336:GLN:NE2	2:B:355:ALA:HB2	1.85	0.91
2:B:360:ALA:HB2	2:B:367:GLN:NE2	1.85	0.91
1:A:108:VAL:HG22	1:A:188:TYR:CD2	2.05	0.90
2:B:72:ARG:HG3	2:B:227:PHE:HZ	1.38	0.89
2:B:241:VAL:CG2	2:B:242:GLN:N	2.34	0.88
2:B:210:LEU:O	2:B:210:LEU:HD23	1.76	0.86
2:B:360:ALA:HB3	2:B:367:GLN:NE2	1.89	0.86
2:B:336:GLN:HE21	2:B:355:ALA:HB2	1.40	0.85
1:A:278:GLN:OE1	1:A:278:GLN:HA	1.75	0.85
1:A:242:GLN:CB	1:A:243:PRO:HD2	2.00	0.83
2:B:425:LEU:HD11	2:B:426:TRP:CD1	2.13	0.83
2:B:360:ALA:CB	2:B:367:GLN:HE21	1.88	0.83
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.59	0.82
2:B:360:ALA:HB1	2:B:361:HIS:C	2.01	0.81
2:B:210:LEU:HD23	2:B:210:LEU:C	2.01	0.81
1:A:292:VAL:HG12	1:A:292:VAL:O	1.78	0.80
2:B:360:ALA:CB	2:B:361:HIS:HA	2.12	0.79
1:A:101:LYS:N	1:A:101:LYS:HD3	1.98	0.78
1:A:108:VAL:CG2	1:A:188:TYR:CD2	2.65	0.78
2:B:239:TRP:CB	2:B:240:THR:HG22	2.13	0.78
1:A:114:ALA:HB1	1:A:214:LEU:HD13	1.66	0.77
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.50	0.77
1:A:90:VAL:HG21	2:B:140:PRO:HB3	1.66	0.77
2:B:80:LEU:O	2:B:84:THR:CG2	2.28	0.76
1:A:309:ILE:HG22	1:A:310:LEU:HD23	1.68	0.76
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.65	0.76
1:A:426:TRP:HZ3	8:A:579:HOH:O	1.69	0.76
2:B:336:GLN:HE21	2:B:355:ALA:HB1	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD12	1:A:93:GLY:H	1.49	0.75
1:A:289:LEU:HD23	1:A:289:LEU:H	1.51	0.75
2:B:211:ARG:HG3	2:B:212:TRP:N	2.02	0.74
2:B:425:LEU:CD1	2:B:426:TRP:CD1	2.71	0.74
2:B:319:TYR:OH	2:B:385:LYS:HE2	1.87	0.74
1:A:260:LEU:HD21	1:A:303:LEU:HD12	1.69	0.74
2:B:72:ARG:HG3	2:B:227:PHE:CZ	2.22	0.73
2:B:423:VAL:HG23	2:B:423:VAL:O	1.86	0.73
2:B:239:TRP:CA	2:B:240:THR:CG2	2.57	0.72
2:B:336:GLN:NE2	2:B:355:ALA:CB	2.47	0.72
1:A:507:GLN:CA	1:A:507:GLN:NE2	2.30	0.72
2:B:241:VAL:HG23	2:B:242:GLN:H	1.54	0.71
2:B:153:TRP:O	2:B:156:SER:HB2	1.90	0.71
2:B:96:HIS:ND1	2:B:97:PRO:HD2	2.05	0.70
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.27	0.70
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.26	0.70
1:A:113:ASP:OD1	1:A:114:ALA:N	2.24	0.70
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.73	0.70
1:A:539:HIS:NE2	3:A:1001:MNK:H12A	2.07	0.69
1:A:255:ASN:OD1	1:A:256:ASP:N	2.25	0.69
2:B:211:ARG:O	2:B:213:GLY:N	2.26	0.69
2:B:353:LYS:HE3	2:B:428:GLN:HE22	1.57	0.69
2:B:360:ALA:HA	2:B:362:THR:H	1.57	0.68
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.75	0.68
1:A:360:ALA:HB1	1:A:514:GLU:HG2	1.73	0.68
1:A:255:ASN:OD1	1:A:255:ASN:C	2.33	0.67
1:A:106:VAL:HG22	1:A:190:GLY:CA	2.24	0.67
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.95	0.67
1:A:539:HIS:CE1	3:A:1001:MNK:H12A	2.30	0.67
1:A:274:ILE:HD11	1:A:310:LEU:HD21	1.78	0.65
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.31	0.65
2:B:211:ARG:CG	2:B:212:TRP:N	2.60	0.65
2:B:156:SER:N	2:B:157:PRO:HD2	2.12	0.65
2:B:6:GLU:CD	2:B:7:THR:H	2.00	0.64
2:B:282:LEU:CD1	2:B:295:LEU:HD23	2.27	0.64
1:A:164:MET:HE2	1:A:164:MET:HA	1.80	0.64
2:B:354:TYR:CB	6:B:1001:DMS:H22	2.28	0.63
1:A:258:GLN:HG2	1:A:259:LYS:N	2.13	0.63
2:B:254:VAL:O	2:B:258:GLN:HG3	1.98	0.63
1:A:242:GLN:CB	1:A:243:PRO:CD	2.58	0.63
1:A:106:VAL:HG22	1:A:190:GLY:HA2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.34	0.62
1:A:89:GLU:N	1:A:89:GLU:OE1	2.30	0.62
2:B:94:ILE:O	2:B:94:ILE:CG1	2.33	0.62
2:B:353:LYS:HE2	2:B:355:ALA:HB2	1.82	0.62
1:A:507:GLN:HE21	1:A:507:GLN:N	1.96	0.61
2:B:320:ASP:OD1	2:B:320:ASP:C	2.39	0.61
1:A:540:LYS:HE3	2:B:265:ASN:OD1	2.01	0.61
1:A:260:LEU:HD23	1:A:279:LEU:HD21	1.83	0.60
1:A:29:GLU:CD	1:A:29:GLU:H	2.03	0.60
1:A:266:TRP:O	1:A:269:GLN:HG2	2.02	0.60
1:A:325:LEU:HD21	1:A:383:TRP:CD2	2.36	0.60
1:A:289:LEU:HD23	1:A:289:LEU:N	2.16	0.59
2:B:108:VAL:CG2	2:B:188:TYR:CE2	2.85	0.59
1:A:247:PRO:O	1:A:307:ARG:NH2	2.34	0.59
2:B:101:LYS:O	2:B:236:PRO:HB3	2.02	0.59
2:B:8:VAL:HG21	2:B:159:ILE:HG12	1.84	0.59
2:B:94:ILE:N	2:B:95:PRO:HD3	2.18	0.59
2:B:85:GLN:HG3	2:B:86:ASP:H	1.68	0.59
2:B:354:TYR:HB3	6:B:1001:DMS:H22	1.84	0.59
2:B:428:GLN:O	2:B:428:GLN:HG3	2.04	0.58
1:A:97:PRO:O	1:A:100:LEU:HG	2.04	0.58
2:B:282:LEU:HD11	2:B:295:LEU:HD23	1.84	0.58
1:A:53:GLU:H	1:A:53:GLU:CD	2.07	0.57
2:B:259:LYS:NZ	8:B:460:HOH:O	2.38	0.57
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.87	0.57
1:A:342:TYR:HA	1:A:349:LEU:HD13	1.85	0.57
1:A:325:LEU:HD11	1:A:349:LEU:HD22	1.86	0.57
1:A:90:VAL:HG22	1:A:90:VAL:O	2.03	0.57
1:A:261:VAL:HG23	1:A:279:LEU:HD23	1.86	0.57
1:A:303:LEU:O	1:A:306:ASN:HB2	2.05	0.57
1:A:424:LYS:HD3	1:A:426:TRP:CH2	2.40	0.57
1:A:277:ARG:NH2	1:A:356:ARG:HE	2.03	0.57
1:A:106:VAL:HG22	1:A:190:GLY:HA3	1.87	0.57
1:A:366:LYS:HE2	1:A:405:TYR:OH	2.05	0.57
1:A:539:HIS:NE2	3:A:1001:MNK:C7	2.68	0.57
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.35	0.57
1:A:295:LEU:HG	1:A:299:ALA:CB	2.34	0.57
2:B:239:TRP:C	2:B:240:THR:HG22	2.24	0.56
2:B:203:GLU:CD	2:B:203:GLU:O	2.44	0.56
2:B:366:LYS:O	2:B:370:GLU:HG2	2.04	0.56
2:B:86:ASP:HA	2:B:154:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.41	0.55
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.70	0.55
2:B:194:GLU:O	2:B:196:GLY:N	2.39	0.55
2:B:360:ALA:HA	2:B:362:THR:N	2.20	0.55
2:B:6:GLU:OE2	2:B:7:THR:N	2.38	0.55
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.40	0.55
2:B:65:LYS:HD2	2:B:227:PHE:CE1	2.42	0.55
2:B:210:LEU:C	2:B:210:LEU:CD2	2.75	0.55
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.89	0.55
1:A:95:PRO:HB3	2:B:136:ASN:O	2.06	0.55
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.41	0.55
1:A:354:TYR:OH	1:A:370:GLU:CB	2.56	0.54
2:B:85:GLN:HG3	2:B:86:ASP:N	2.21	0.54
2:B:314:VAL:HG12	2:B:315:HIS:N	2.22	0.54
2:B:360:ALA:CB	2:B:361:HIS:CA	2.68	0.54
2:B:399:GLU:CD	7:B:429:EDO:H11	2.28	0.54
1:A:90:VAL:CG2	2:B:140:PRO:HB3	2.37	0.54
1:A:354:TYR:OH	1:A:370:GLU:HB3	2.08	0.54
2:B:156:SER:H	2:B:157:PRO:HD2	1.70	0.54
1:A:345:PRO:O	1:A:346:PHE:HB2	2.07	0.54
2:B:74:LEU:HD12	2:B:75:VAL:N	2.22	0.54
1:A:354:TYR:OH	1:A:370:GLU:OE1	2.26	0.53
1:A:360:ALA:CB	1:A:514:GLU:HG2	2.39	0.53
2:B:85:GLN:O	2:B:87:PHE:HD1	1.92	0.53
2:B:101:LYS:O	2:B:236:PRO:CB	2.57	0.53
1:A:103:LYS:HE2	1:A:191:SER:HA	1.90	0.52
1:A:22:LYS:O	1:A:22:LYS:HG3	2.08	0.52
1:A:539:HIS:NE2	3:A:1001:MNK:C12	2.73	0.52
1:A:29:GLU:CD	1:A:29:GLU:N	2.62	0.52
1:A:328:GLU:HG2	1:A:390:LYS:CB	2.34	0.52
2:B:63:ILE:HG13	2:B:63:ILE:O	2.08	0.52
1:A:237:ASP:C	1:A:238:LYS:HG3	2.30	0.52
1:A:454:LYS:NZ	1:A:554:ALA:HA	2.25	0.52
1:A:134:SER:HA	8:A:578:HOH:O	2.09	0.52
1:A:253:THR:O	1:A:254:VAL:C	2.48	0.52
1:A:553:SER:O	1:A:554:ALA:CB	2.58	0.51
2:B:96:HIS:CE1	2:B:97:PRO:HD2	2.44	0.51
2:B:96:HIS:CG	2:B:97:PRO:HD2	2.45	0.51
1:A:252:TRP:HB3	1:A:257:ILE:HD11	1.92	0.51
2:B:108:VAL:CG2	2:B:188:TYR:CD2	2.93	0.51
2:B:423:VAL:HA	2:B:426:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:O	1:A:195:ILE:HG13	2.10	0.51
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.91	0.51
2:B:425:LEU:HD12	2:B:426:TRP:CD1	2.45	0.51
1:A:539:HIS:O	1:A:540:LYS:HD3	2.11	0.51
2:B:425:LEU:HD11	2:B:426:TRP:NE1	2.25	0.51
1:A:255:ASN:HB2	1:A:289:LEU:HD13	1.94	0.50
1:A:544:GLY:CA	2:B:286:THR:HG22	2.37	0.50
1:A:404:GLU:OE1	1:A:431:LYS:HE3	2.11	0.50
2:B:85:GLN:O	2:B:87:PHE:CD1	2.65	0.50
2:B:86:ASP:OD1	2:B:86:ASP:O	2.30	0.50
1:A:307:ARG:HH11	1:A:307:ARG:CG	2.19	0.50
2:B:212:TRP:HE3	2:B:212:TRP:O	1.95	0.49
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.95	0.49
1:A:253:THR:O	1:A:256:ASP:N	2.44	0.49
2:B:332:GLN:OE1	2:B:424:LYS:HE3	2.12	0.49
1:A:92:LEU:CD1	1:A:93:GLY:N	2.65	0.49
1:A:202:ILE:O	1:A:206:ARG:HG3	2.11	0.49
2:B:203:GLU:O	2:B:203:GLU:OE2	2.31	0.49
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.43	0.49
2:B:208:HIS:O	2:B:208:HIS:ND1	2.44	0.49
1:A:325:LEU:HD12	1:A:343:GLN:HG3	1.95	0.49
2:B:9:PRO:O	2:B:10:VAL:CG2	2.60	0.49
1:A:164:MET:HB3	1:A:182:GLN:HE22	1.77	0.49
1:A:103:LYS:HE2	1:A:191:SER:CA	2.43	0.49
1:A:307:ARG:HG3	1:A:307:ARG:NH1	2.25	0.49
1:A:237:ASP:OD2	1:A:238:LYS:HE3	2.12	0.49
1:A:91:GLN:HG3	1:A:91:GLN:O	2.12	0.48
1:A:282:LEU:HD11	1:A:299:ALA:HB2	1.95	0.48
1:A:292:VAL:O	1:A:292:VAL:CG1	2.51	0.48
1:A:417:VAL:O	1:A:417:VAL:HG13	2.13	0.48
1:A:257:ILE:CG2	1:A:283:LEU:HD21	2.43	0.48
2:B:196:GLY:O	2:B:200:THR:HG23	2.12	0.48
1:A:406:TRP:CE2	1:A:407:GLN:HG3	2.48	0.48
1:A:475:GLN:NE2	1:A:501:TYR:CE1	2.82	0.48
2:B:46:LYS:HE2	2:B:116:PHE:HB3	1.96	0.48
1:A:217:PRO:O	1:A:219:LYS:N	2.47	0.48
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.95	0.48
1:A:255:ASN:CG	1:A:256:ASP:N	2.67	0.48
1:A:307:ARG:CG	1:A:307:ARG:NH1	2.77	0.48
2:B:235:HIS:HB3	2:B:238:LYS:HG3	1.95	0.48
1:A:308:GLU:O	1:A:308:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.49	0.47
1:A:365:VAL:HG11	1:A:401:TRP:CD1	2.49	0.47
1:A:457:TYR:CD1	1:A:457:TYR:C	2.88	0.47
2:B:12:LEU:HD11	2:B:127:TYR:CE2	2.50	0.47
1:A:511:ASP:OD1	1:A:511:ASP:C	2.52	0.47
1:A:113:ASP:OD1	1:A:113:ASP:C	2.52	0.47
1:A:284:ARG:O	1:A:284:ARG:HG2	2.15	0.47
1:A:289:LEU:HA	1:A:290:THR:HA	1.66	0.47
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.50	0.47
2:B:240:THR:HG23	2:B:240:THR:O	2.14	0.47
1:A:108:VAL:HG21	1:A:188:TYR:CE2	2.50	0.47
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.97	0.47
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.35	0.47
1:A:360:ALA:O	1:A:513:SER:HA	2.15	0.47
1:A:542:ILE:O	1:A:546:GLU:HG2	2.15	0.47
1:A:543:GLY:N	2:B:283:LEU:O	2.48	0.47
1:A:108:VAL:CG2	1:A:188:TYR:CE2	2.97	0.47
2:B:10:VAL:HG13	2:B:87:PHE:CE1	2.50	0.47
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.50	0.47
2:B:206:ARG:O	2:B:210:LEU:N	2.42	0.47
1:A:553:SER:O	1:A:554:ALA:HB2	2.15	0.46
2:B:167:ILE:HG12	2:B:212:TRP:CE3	2.49	0.46
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.44	0.46
1:A:191:SER:OG	1:A:198:HIS:ND1	2.44	0.46
1:A:503:LEU:O	1:A:507:GLN:HB2	2.15	0.46
2:B:394:GLN:NE2	2:B:396:GLU:OE1	2.48	0.46
1:A:107:THR:OG1	1:A:198:HIS:NE2	2.47	0.46
1:A:289:LEU:HB2	1:A:290:THR:HG22	1.98	0.46
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.51	0.46
2:B:6:GLU:CG	2:B:7:THR:N	2.79	0.46
1:A:489:SER:O	1:A:528:LYS:NZ	2.49	0.46
1:A:295:LEU:HG	1:A:299:ALA:HB1	1.97	0.46
1:A:450:THR:O	1:A:451:LYS:HB2	2.15	0.46
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.98	0.45
1:A:295:LEU:HG	1:A:299:ALA:HB3	1.97	0.45
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.52	0.45
1:A:543:GLY:C	1:A:545:ASN:H	2.19	0.45
2:B:279:LEU:O	2:B:282:LEU:HB2	2.17	0.45
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.81	0.45
2:B:374:LYS:HD2	6:B:1001:DMS:C1	2.46	0.45
1:A:426:TRP:HB3	1:A:526:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:GLU:C	2:B:196:GLY:H	2.20	0.45
1:A:255:ASN:CB	1:A:289:LEU:HD13	2.47	0.45
1:A:89:GLU:O	1:A:89:GLU:HG2	2.17	0.45
1:A:92:LEU:CD1	1:A:93:GLY:H	2.25	0.45
1:A:391:LEU:C	1:A:417:VAL:HG12	2.37	0.45
2:B:211:ARG:C	2:B:213:GLY:N	2.69	0.45
1:A:277:ARG:HH21	1:A:356:ARG:NE	2.15	0.45
1:A:109:LEU:O	1:A:187:LEU:N	2.35	0.44
2:B:10:VAL:CG2	2:B:159:ILE:HD11	2.48	0.44
1:A:216:THR:HA	1:A:217:PRO:HD3	1.35	0.44
1:A:257:ILE:CB	1:A:283:LEU:HD21	2.47	0.44
2:B:10:VAL:HG13	2:B:87:PHE:CZ	2.52	0.44
2:B:6:GLU:CD	2:B:7:THR:N	2.68	0.44
2:B:94:ILE:N	2:B:95:PRO:CD	2.78	0.44
2:B:156:SER:N	2:B:157:PRO:CD	2.79	0.44
2:B:360:ALA:CA	2:B:362:THR:H	2.27	0.44
1:A:325:LEU:HD12	1:A:343:GLN:CG	2.48	0.44
2:B:66:LYS:O	2:B:68:SER:N	2.49	0.44
1:A:289:LEU:H	1:A:289:LEU:CD2	2.18	0.44
1:A:426:TRP:CZ3	8:A:579:HOH:O	2.54	0.44
1:A:89:GLU:O	1:A:89:GLU:CG	2.66	0.44
1:A:238:LYS:NZ	8:A:574:HOH:O	2.46	0.44
1:A:277:ARG:NH2	1:A:356:ARG:NE	2.65	0.44
2:B:66:LYS:C	2:B:68:SER:N	2.71	0.44
1:A:543:GLY:HA3	2:B:285:GLY:O	2.17	0.44
2:B:208:HIS:O	2:B:212:TRP:HB2	2.18	0.44
1:A:135:ILE:O	1:A:136:ASN:HB2	2.17	0.44
2:B:65:LYS:HD3	2:B:230:MET:CE	2.48	0.44
2:B:211:ARG:C	2:B:213:GLY:H	2.21	0.44
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.00	0.43
1:A:240:THR:OG1	1:A:241:VAL:N	2.51	0.43
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.53	0.43
2:B:103:LYS:O	2:B:104:LYS:C	2.57	0.43
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.54	0.43
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.43
1:A:503:LEU:HD22	1:A:535:TRP:HB2	2.00	0.43
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.99	0.43
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.33	0.43
2:B:13:LYS:HA	2:B:14:PRO:HD3	1.80	0.43
1:A:540:LYS:HD3	1:A:540:LYS:HA	1.77	0.43
2:B:9:PRO:C	2:B:10:VAL:HG23	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:HA	1:A:220:LYS:HD3	1.83	0.42
2:B:395:LYS:HB2	2:B:416:PHE:CD1	2.54	0.42
1:A:325:LEU:HD11	1:A:349:LEU:CD2	2.47	0.42
1:A:540:LYS:O	2:B:280:SER:OG	2.21	0.42
2:B:360:ALA:CA	2:B:362:THR:N	2.82	0.42
1:A:103:LYS:HE2	1:A:191:SER:N	2.34	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.19	0.42
1:A:198:HIS:O	1:A:202:ILE:HG12	2.19	0.42
2:B:257:ILE:O	2:B:261:VAL:HG23	2.20	0.42
1:A:118:VAL:HG11	1:A:149:LEU:HD11	2.02	0.41
3:A:1001:MNK:H9	3:A:1001:MNK:H8	1.85	0.41
1:A:92:LEU:HD12	1:A:93:GLY:CA	2.47	0.41
2:B:122:GLU:HA	2:B:125:ARG:HG3	2.03	0.41
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.20	0.41
2:B:282:LEU:HD12	2:B:295:LEU:HD23	2.02	0.41
2:B:395:LYS:O	2:B:399:GLU:HG3	2.20	0.41
1:A:424:LYS:HE2	1:A:426:TRP:CE3	2.56	0.41
1:A:299:ALA:O	1:A:303:LEU:HB3	2.20	0.41
2:B:94:ILE:O	2:B:95:PRO:O	2.38	0.41
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.56	0.41
1:A:286:THR:OG1	1:A:287:LYS:N	2.54	0.41
4:A:555:T27:H17	4:A:555:T27:N3	2.36	0.41
2:B:38:CYS:HB3	2:B:144:TYR:CE1	2.55	0.41
2:B:78:ARG:O	2:B:82:LYS:HG3	2.20	0.41
2:B:395:LYS:HG3	2:B:416:PHE:CE1	2.56	0.41
2:B:239:TRP:HA	2:B:240:THR:CB	2.49	0.41
1:A:181:TYR:HE2	1:A:183:TYR:HB2	1.79	0.41
1:A:194:GLU:HG3	1:A:197:GLN:HG2	2.01	0.41
2:B:227:PHE:HB3	2:B:229:TRP:HE1	1.86	0.41
2:B:358:ARG:HA	2:B:358:ARG:HD2	1.58	0.41
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.86	0.41
2:B:358:ARG:HD2	2:B:359:GLY:N	2.36	0.41
1:A:324:ASP:O	1:A:343:GLN:HG2	2.21	0.40
2:B:241:VAL:O	2:B:242:GLN:HG2	2.20	0.40
2:B:360:ALA:CB	2:B:367:GLN:HE22	2.27	0.40
1:A:167:ILE:HG23	1:A:212:TRP:CZ3	2.56	0.40
2:B:182:GLN:HB2	2:B:187:LEU:HD12	2.04	0.40
1:A:39:THR:O	1:A:43:LYS:HG3	2.21	0.40
1:A:253:THR:O	1:A:255:ASN:N	2.54	0.40
1:A:329:ILE:O	1:A:392:PRO:HD3	2.22	0.40
2:B:393:ILE:HG12	2:B:394:GLN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:TRP:O	2:B:407:GLN:HG2	2.22	0.40
2:B:422:LEU:C	2:B:424:LYS:H	2.25	0.40
1:A:269:GLN:HA	1:A:351:THR:O	2.21	0.40
1:A:451:LYS:HE2	1:A:451:LYS:HB3	1.78	0.40
2:B:160:PHE:CE2	2:B:164:MET:HB2	2.56	0.40
2:B:161:GLN:O	2:B:162:SER:C	2.60	0.40
1:A:106:VAL:HA	1:A:190:GLY:HA2	2.04	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	553/555 (100%)	521 (94%)	31 (6%)	1 (0%)	47 73
2	B	401/423 (95%)	369 (92%)	31 (8%)	1 (0%)	47 73
All	All	954/978 (98%)	890 (93%)	62 (6%)	2 (0%)	47 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	212	TRP
1	A	254	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	494/494 (100%)	460 (93%)	34 (7%)	15 35
2	B	370/385 (96%)	338 (91%)	32 (9%)	10 24
All	All	864/879 (98%)	798 (92%)	66 (8%)	13 30

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	16	MET
1	A	100	LEU
1	A	101	LYS
1	A	103	LYS
1	A	105	SER
1	A	107	THR
1	A	113	ASP
1	A	151	GLN
1	A	174	GLN
1	A	177	ASP
1	A	182	GLN
1	A	193	LEU
1	A	195	ILE
1	A	197	GLN
1	A	238	LYS
1	A	253	THR
1	A	255	ASN
1	A	258	GLN
1	A	261	VAL
1	A	286	THR
1	A	289	LEU
1	A	295	LEU
1	A	298	GLU
1	A	303	LEU
1	A	324	ASP
1	A	353	LYS
1	A	431	LYS
1	A	459	THR
1	A	463	ARG
1	A	476	LYS
1	A	480	GLN
1	A	507	GLN
1	A	509	GLN
2	B	55	PRO

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Mol	Chain	Res	Type
2	B	67	ASP
2	B	68	SER
2	B	69	THR
2	B	70	LYS
2	B	72	ARG
2	B	84	THR
2	B	85	GLN
2	B	94	ILE
2	B	126	LYS
2	B	133	PRO
2	B	154	LYS
2	B	156	SER
2	B	162	SER
2	B	163	SER
2	B	177	ASP
2	B	210	LEU
2	B	212	TRP
2	B	227	PHE
2	B	233	GLU
2	B	241	VAL
2	B	244	ILE
2	B	281	LYS
2	B	284	ARG
2	B	330	GLN
2	B	356	ARG
2	B	358	ARG
2	B	394	GLN
2	B	404	GLU
2	B	414	TRP
2	B	423	VAL
2	B	424	LYS

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

Mol	Chain	Res	Type
1	A	136	ASN
1	A	147	ASN
1	A	174	GLN
1	A	182	GLN
1	A	334	GLN
1	A	475	GLN
1	A	507	GLN

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Mol	Chain	Res	Type
1	A	509	GLN
1	A	524	GLN
2	B	151	GLN
2	B	161	GLN
2	B	278	GLN
2	B	330	GLN
2	B	336	GLN
2	B	340	GLN
2	B	373	GLN
2	B	394	GLN
2	B	428	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
7	EDO	B	429	-	3,3,3	0.37	0	2,2,2	0.52	0
3	MNK	A	1001	5	17,19,19	1.82	4 (23%)	20,28,28	2.63	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	T27	A	555	-	30,30,30	2.18	12 (40%)	39,40,40	1.06	3 (7%)
6	DMS	B	1001	-	3,3,3	0.72	0	3,3,3	1.06	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
7	EDO	B	429	-	-	1/1/1/1	-
3	MNK	A	1001	5	-	4/4/13/13	0/2/2/2
4	T27	A	555	-	-	2/13/14/14	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	555	T27	C6-C5	4.87	1.47	1.40
4	A	555	T27	C17-C16	4.83	1.47	1.39
3	A	1001	MNK	C9-C6	4.26	1.57	1.51
3	A	1001	MNK	C14-C13	3.53	1.48	1.34
4	A	555	T27	C6-C1	3.45	1.45	1.40
3	A	1001	MNK	O2-C2	3.16	1.30	1.23
4	A	555	T27	C15-C16	3.02	1.44	1.39
4	A	555	T27	C12-N4	2.93	1.42	1.36
4	A	555	T27	C18-C17	2.63	1.43	1.38
4	A	555	T27	C2-C3	2.57	1.44	1.39
4	A	555	T27	C2-C1	2.55	1.43	1.39
4	A	555	T27	C9-N2	2.34	1.39	1.34
4	A	555	T27	C14-C13	2.33	1.44	1.39
3	A	1001	MNK	C10-C13	2.29	1.57	1.51
4	A	555	T27	C4-C5	2.27	1.42	1.39
4	A	555	T27	C15-C14	2.26	1.42	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	MNK	C10-C9-C6	6.97	127.93	110.69
3	A	1001	MNK	C11-C12-C7	5.23	124.00	111.56
3	A	1001	MNK	C4-C5-C6	4.65	132.55	123.90
4	A	555	T27	C5-C6-N1	3.02	124.95	119.34
3	A	1001	MNK	C8-C5-C4	-2.72	111.93	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	555	T27	C9-C10-C11	-2.58	115.07	116.76
3	A	1001	MNK	C8-C5-C6	-2.31	115.52	120.71
3	A	1001	MNK	C12-C11-C10	2.20	119.60	112.62
4	A	555	T27	C2-C1-C6	2.05	120.63	118.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	429	EDO	O1-C1-C2-O2
3	A	1001	MNK	C11-C10-C13-C14
3	A	1001	MNK	C11-C10-C13-C15
3	A	1001	MNK	C9-C10-C13-C14
3	A	1001	MNK	C9-C10-C13-C15
4	A	555	T27	C20-C21-C3-C2
4	A	555	T27	C20-C21-C3-C4

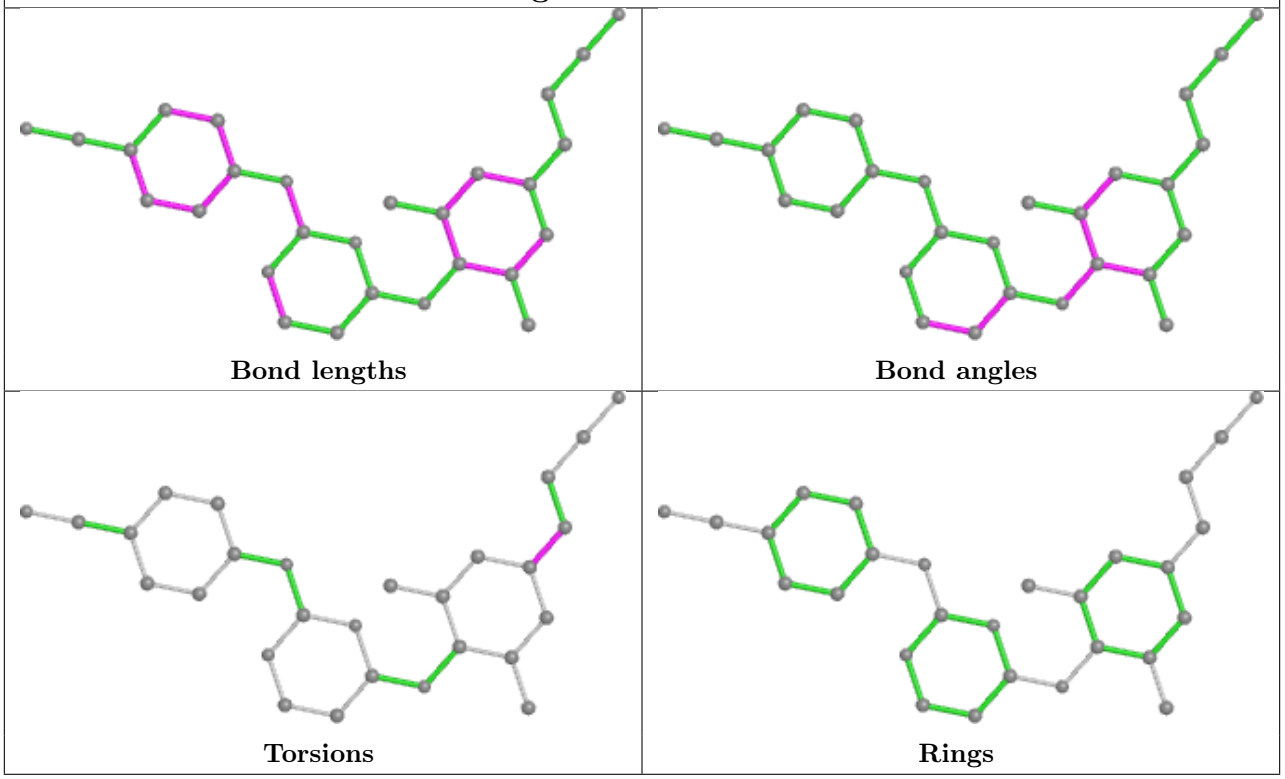
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	429	EDO	1	0
3	A	1001	MNK	5	0
4	A	555	T27	1	0
6	B	1001	DMS	3	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 then 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.

Ligand T27 A 555



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	555/555 (100%)	0.60	58 (10%)	6	4	30, 72, 129, 158	0
2	B	407/423 (96%)	0.59	37 (9%)	9	7	31, 69, 128, 143	0
All	All	962/978 (98%)	0.60	95 (9%)	7	5	30, 71, 128, 158	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	LYS	7.2
1	A	66	LYS	6.9
1	A	220	LYS	6.6
1	A	290	THR	6.4
1	A	252	TRP	5.9
1	A	218	ASP	5.8
2	B	355	ALA	5.5
2	B	230	MET	5.5
1	A	277	ARG	5.5
1	A	284	ARG	5.4
2	B	229	TRP	5.3
1	A	358	ARG	5.3
1	A	295	LEU	5.2
1	A	222	GLN	5.1
1	A	221	HIS	5.1
1	A	70	LYS	5.0
1	A	254	VAL	4.9
1	A	292	VAL	4.9
2	B	202	ILE	4.8
2	B	197	GLN	4.7
2	B	173	LYS	4.6
2	B	315	HIS	4.6
2	B	67	ASP	4.6
2	B	166	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	4.3
1	A	285	GLY	4.3
1	A	250	ASP	4.3
1	A	24	TRP	4.2
2	B	69	THR	4.2
1	A	288	ALA	4.2
1	A	279	LEU	4.1
1	A	278	GLN	4.1
1	A	91	GLN	4.1
1	A	117	SER	4.1
1	A	64	LYS	4.1
1	A	257	ILE	4.1
1	A	286	THR	4.1
1	A	69	THR	3.9
2	B	209	LEU	3.9
1	A	74	LEU	3.8
2	B	65	LYS	3.7
1	A	183	TYR	3.7
1	A	276	VAL	3.7
2	B	6	GLU	3.6
1	A	256	ASP	3.6
1	A	116	PHE	3.5
2	B	198	HIS	3.5
1	A	112	GLY	3.5
1	A	71	TRP	3.4
1	A	300	GLU	3.3
2	B	66	LYS	3.3
2	B	357	MET	3.2
1	A	283	LEU	3.1
1	A	301	LEU	3.1
1	A	62	ALA	3.0
2	B	212	TRP	3.0
2	B	169	GLU	2.9
1	A	289	LEU	2.9
2	B	227	PHE	2.8
1	A	65	LYS	2.8
2	B	206	ARG	2.8
2	B	13	LYS	2.8
2	B	168	LEU	2.8
1	A	246	LEU	2.7
2	B	231	GLY	2.7
1	A	219	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	170	PRO	2.6
2	B	284	ARG	2.6
1	A	244	ILE	2.6
1	A	63	ILE	2.5
1	A	260	LEU	2.5
2	B	240	THR	2.5
1	A	184	MET	2.5
2	B	171	PHE	2.5
2	B	85	GLN	2.5
2	B	195	ILE	2.5
2	B	11	LYS	2.5
2	B	191	SER	2.5
2	B	193	LEU	2.4
1	A	346	PHE	2.4
2	B	180	ILE	2.4
1	A	109	LEU	2.4
1	A	302	GLU	2.3
1	A	77	PHE	2.3
2	B	210	LEU	2.2
2	B	356	ARG	2.2
1	A	72	ARG	2.2
1	A	223	LYS	2.2
1	A	298	GLU	2.1
2	B	421	PRO	2.1
1	A	114	ALA	2.1
1	A	89	GLU	2.1
1	A	293	ILE	2.1
2	B	228	LEU	2.0
1	A	245	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

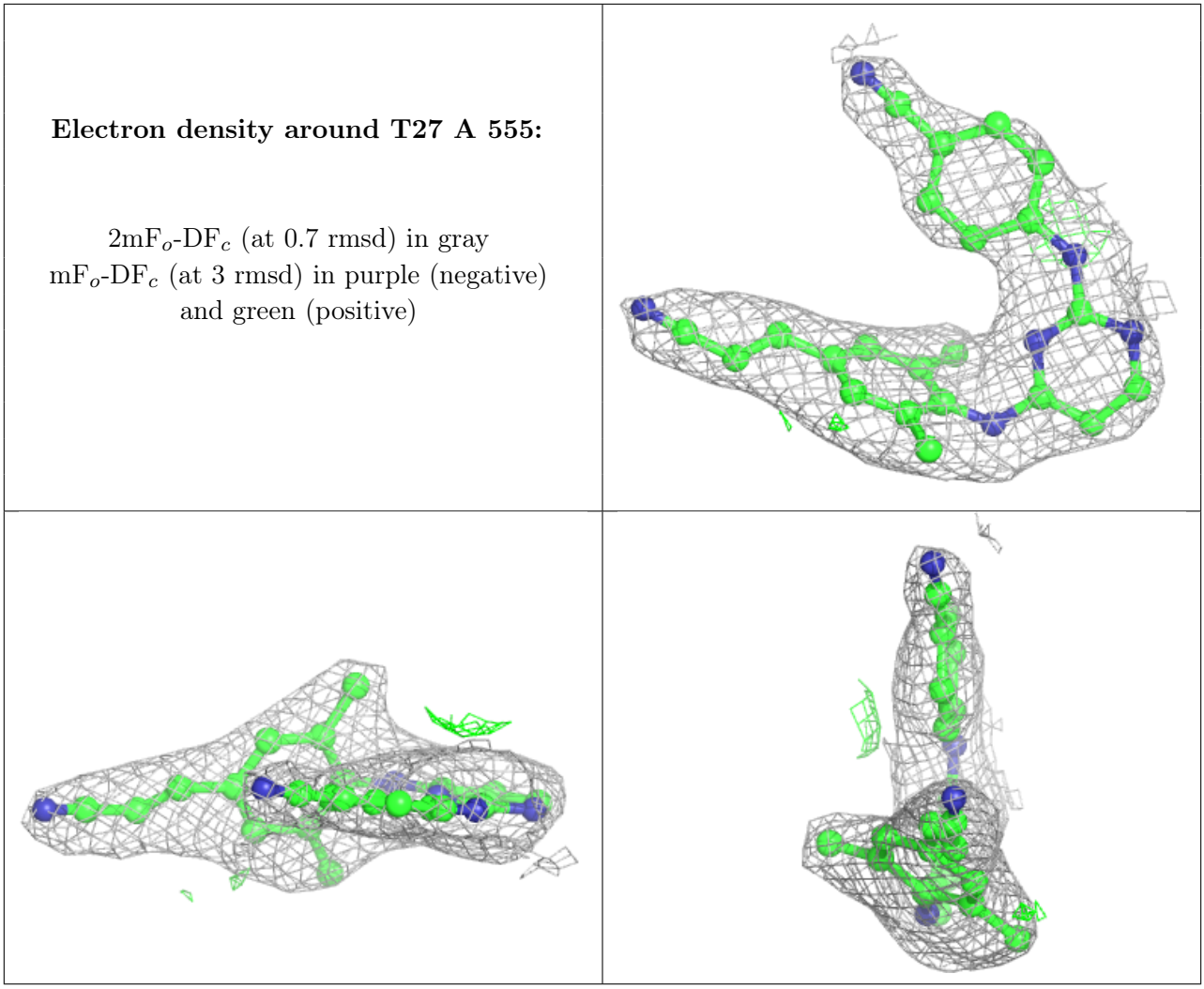
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MNK	A	1001	18/18	0.83	0.28	83,93,98,100	0
4	T27	A	555	28/28	0.90	0.22	60,68,74,75	0
5	MN	A	556	1/1	0.91	0.14	79,79,79,79	0
6	DMS	B	1001	4/4	0.92	0.29	106,107,107,111	0
7	EDO	B	429	4/4	0.93	0.27	64,67,70,71	0
5	MN	A	557	1/1	0.98	0.19	56,56,56,56	0

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

Electron density around T27 A 555:

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



6.5 Other polymers (i)

There are no such residues in this entry.