



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:04 am BST

PDB ID : 3QO9
Title : Crystal structure of HIV-1 Reverse Transcriptase (RT) in complex with TSAO-T, a non-nucleoside RT inhibitor (NNRTI)
Authors : Das, K.; Arnold, E.
Deposited on : 2011-02-09
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

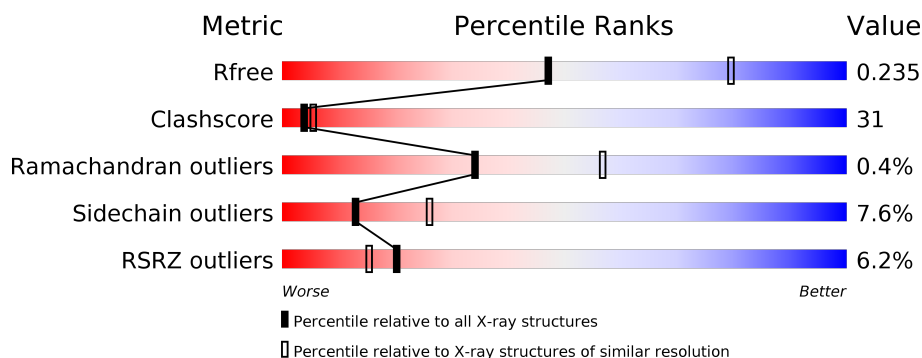
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	557	<div> <div>6%</div> <div> <div></div> <div>53%</div> <div>41%</div> <div>5%</div> </div> </div>
2	B	428	<div> <div>7%</div> <div> <div></div> <div>50%</div> <div>41%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7987 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
1	A	553	Total	C	N	O	S	0	0	0
			4500	2912	749	832	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P03366
A	0	VAL	-	EXPRESSION TAG	UNP P03366
A	160	SER	PHE	ENGINEERED MUTATION	UNP P03366
A	280	SER	CYS	ENGINEERED MUTATION	UNP P03366

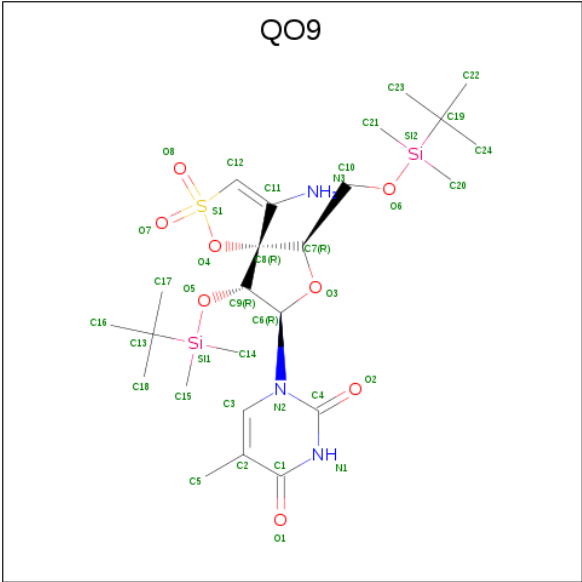
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3413	2225	564	617	7			

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 1-[(5R,6R,8R,9R)-4-amino-9-{[tert-butyl(dimethyl)silyl]oxy}-6-([tert-butyl(dimethyl)silyl]oxy)methyl]-2,2-dioxido-1,7-dioxo-2-thiaspiro[4.4]non-3-en-8-yl]-5-methylpyrimidine-2,4(1H,3H)-dione (three-letter code: QO9) (formula: C₂₄H₄₃N₃O₈SSi₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	Si	0	0
			38	24	3	8	1	2		

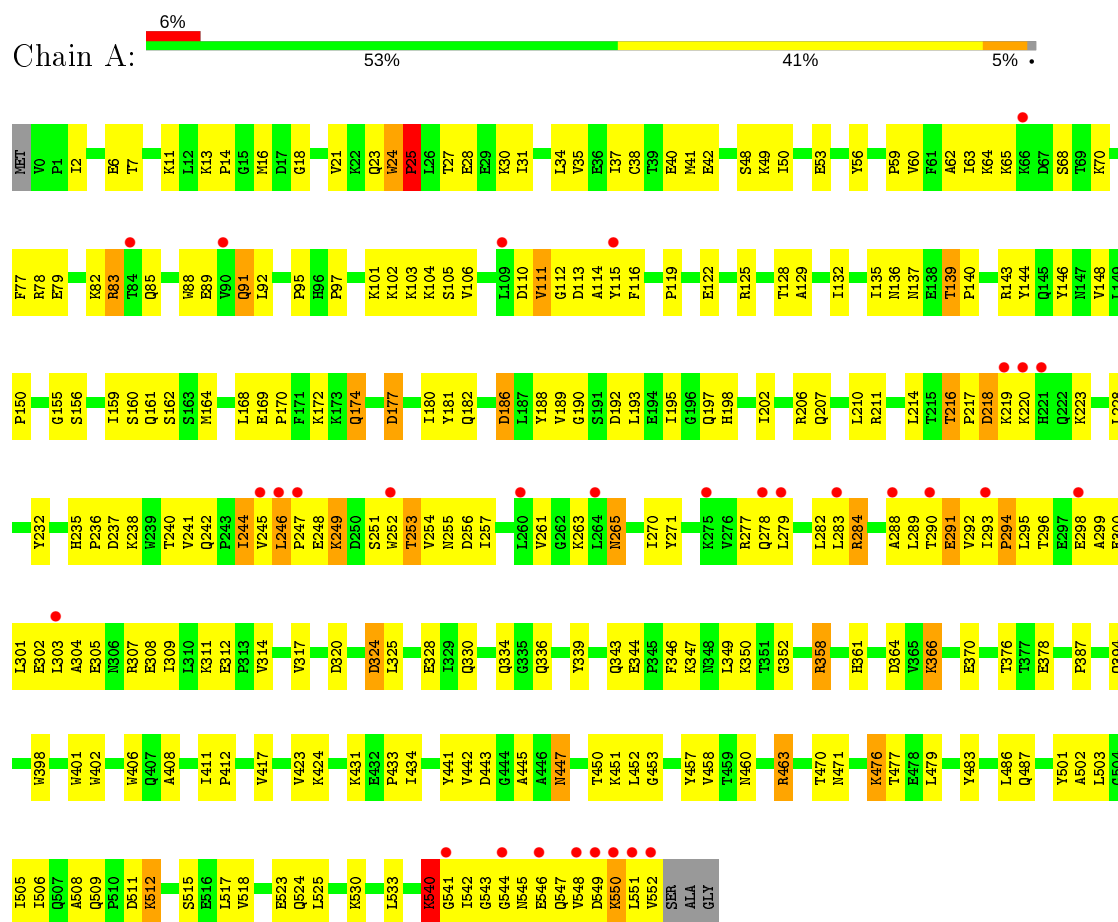
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	11	Total	O	0	0
			11	11		

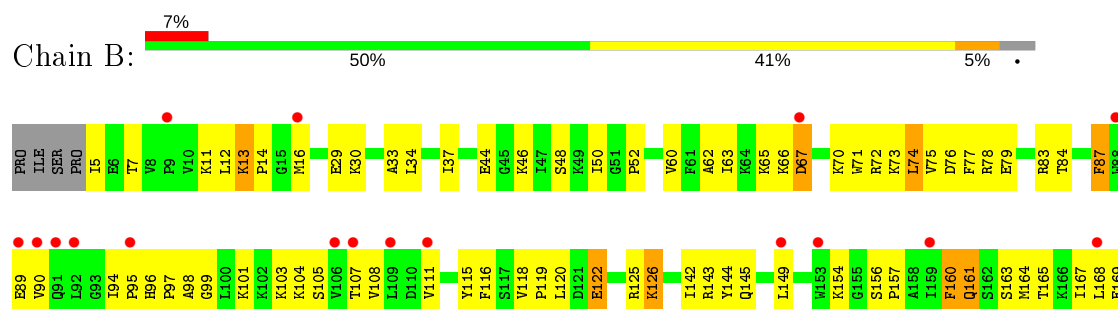
3 Residue-property plots [i](#)

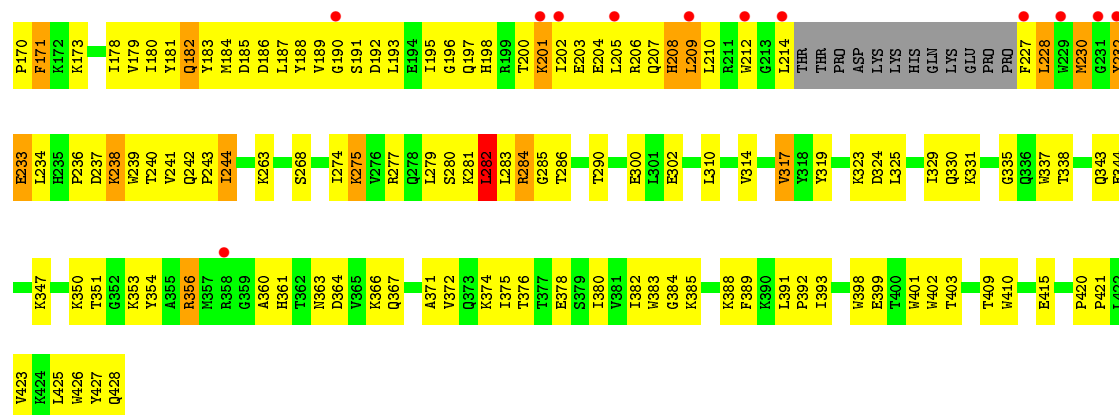
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



- Molecule 2: p51 RT





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.76Å 72.59Å 108.97Å 90.00° 98.75° 90.00°	Depositor
Resolution (Å)	48.27 – 2.60 48.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.27-2.60) 96.5 (48.27-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.286 0.240 , 0.235	Depositor DCC
R_{free} test set	1465 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7987	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: QO9

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	0.44	0/4617	0.73	4/6274 (0.1%)
2	B	0.43	0/3511	0.73	1/4768 (0.0%)
All	All	0.44	0/8128	0.73	5/11042 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	LYS	N-CA-C	-6.21	94.22	111.00
1	A	218	ASP	N-CA-C	-6.10	94.52	111.00
1	A	25	PRO	N-CA-C	-5.43	97.99	112.10
2	B	282	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	540	LYS	N-CA-C	-5.21	96.92	111.00

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	4500	0	4565	279	0
2	B	3413	0	3443	224	0
3	A	38	0	31	3	0
4	A	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	0	0	0	0
All	All	7987	0	8039	490	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 31.

All (490) 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:46:LYS:HE3	2:B:116:PHE:HB3	1.20	1.16
1:A:253:THR:HG23	1:A:256:ASP:HB2	1.35	1.05
1:A:447:ASN:HB3	1:A:450:THR:HG22	1.40	1.03
1:A:68:SER:HB3	1:A:70:LYS:HE3	1.41	1.02
2:B:232:TYR:HE2	2:B:374:LYS:HZ1	1.04	0.98
2:B:178:ILE:HD11	2:B:201:LYS:HD3	1.44	0.97
2:B:111:VAL:HG11	2:B:187:LEU:HD12	1.43	0.96
2:B:44:GLU:HG3	2:B:46:LYS:HG2	1.49	0.94
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.50	0.94
2:B:193:LEU:HB3	2:B:197:GLN:HG3	1.50	0.93
1:A:541:GLY:HA2	1:A:546:GLU:OE1	1.72	0.90
2:B:170:PRO:HG3	2:B:212:TRP:HE1	1.36	0.90
1:A:40:GLU:HG3	1:A:41:MET:N	1.88	0.89
2:B:170:PRO:HG2	2:B:208:HIS:NE2	1.87	0.89
1:A:217:PRO:HG2	1:A:219:LYS:HB2	1.55	0.89
1:A:128:THR:HG21	1:A:146:TYR:HB2	1.54	0.88
2:B:282:LEU:H	2:B:282:LEU:HD12	1.39	0.87
1:A:550:LYS:HB3	1:A:550:LYS:NZ	1.90	0.86
1:A:542:ILE:HG23	2:B:283:LEU:HB3	1.58	0.86
2:B:371:ALA:O	2:B:375:ILE:HG13	1.74	0.86
2:B:197:GLN:NE2	2:B:201:LYS:HB2	1.92	0.85
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.56	0.85
2:B:63:ILE:HD13	2:B:74:LEU:HD23	1.56	0.84
1:A:544:GLY:O	1:A:548:VAL:N	2.08	0.84
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.60	0.84
1:A:502:ALA:O	1:A:506:ILE:HG22	1.78	0.84
1:A:253:THR:H	1:A:256:ASP:CB	1.91	0.83
1:A:544:GLY:O	1:A:548:VAL:HG23	1.79	0.83
2:B:197:GLN:HE22	2:B:201:LYS:HB2	1.41	0.82
1:A:441:TYR:CB	1:A:544:GLY:HA3	2.10	0.81
1:A:543:GLY:HA2	2:B:285:GLY:O	1.79	0.81
2:B:363:ASN:O	2:B:367:GLN:HG3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:HB3	1:A:450:THR:CG2	2.12	0.80
1:A:254:VAL:HG21	1:A:288:ALA:O	1.81	0.80
2:B:46:LYS:HE3	2:B:116:PHE:CB	2.09	0.79
1:A:441:TYR:HB2	1:A:544:GLY:HA3	1.62	0.79
1:A:255:ASN:HB2	1:A:289:LEU:HD23	1.65	0.78
1:A:255:ASN:HB2	1:A:289:LEU:CD2	2.13	0.77
2:B:198:HIS:O	2:B:201:LYS:HB3	1.85	0.77
2:B:353:LYS:HZ2	2:B:428:GLN:HE21	1.30	0.77
2:B:87:PHE:CD2	2:B:87:PHE:N	2.51	0.77
2:B:104:LYS:O	2:B:236:PRO:HD2	1.84	0.77
2:B:87:PHE:HD2	2:B:87:PHE:N	1.83	0.77
1:A:283:LEU:HB2	1:A:284:ARG:HH12	1.50	0.77
1:A:284:ARG:NE	1:A:358:ARG:HH22	1.83	0.76
2:B:241:VAL:HG13	2:B:351:THR:HG23	1.67	0.76
1:A:458:VAL:HG13	1:A:548:VAL:HG22	1.67	0.76
2:B:181:TYR:HB3	2:B:188:TYR:HB2	1.69	0.75
2:B:87:PHE:HD2	2:B:87:PHE:H	1.36	0.74
1:A:328:GLU:HG2	1:A:330:GLN:NE2	2.04	0.73
1:A:293:ILE:HG23	1:A:294:PRO:HD2	1.70	0.72
1:A:443:ASP:HB3	1:A:548:VAL:CG1	2.19	0.72
2:B:279:LEU:HA	2:B:282:LEU:HD11	1.72	0.72
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.25	0.72
1:A:13:LYS:HB2	1:A:16:MET:SD	2.31	0.71
1:A:111:VAL:O	1:A:111:VAL:HG13	1.90	0.71
1:A:450:THR:HG23	1:A:452:LEU:H	1.56	0.71
1:A:517:LEU:HA	4:A:580:HOH:O	1.89	0.70
1:A:254:VAL:HB	1:A:289:LEU:HA	1.72	0.70
2:B:353:LYS:NZ	2:B:428:GLN:HE21	1.88	0.70
2:B:244:ILE:HB	2:B:310:LEU:HD13	1.73	0.70
1:A:253:THR:H	1:A:256:ASP:HB3	1.57	0.69
2:B:164:MET:CE	2:B:187:LEU:HD11	2.22	0.69
1:A:447:ASN:CB	1:A:450:THR:HG22	2.20	0.69
1:A:511:ASP:O	1:A:512:LYS:HE3	1.92	0.68
2:B:13:LYS:HB3	2:B:16:MET:SD	2.33	0.68
1:A:136:ASN:O	1:A:137:ASN:HB2	1.94	0.68
1:A:541:GLY:HA2	1:A:546:GLU:CD	2.14	0.68
1:A:328:GLU:HG2	1:A:330:GLN:HE21	1.58	0.67
1:A:23:GLN:HE21	1:A:24:TRP:HB2	1.59	0.67
1:A:541:GLY:C	1:A:546:GLU:HB2	2.14	0.67
1:A:442:VAL:O	1:A:545:ASN:ND2	2.27	0.67
2:B:268:SER:HB3	2:B:274:ILE:HB	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:ASP:CG	2:B:409:THR:HG21	2.15	0.66
1:A:344:GLU:OE2	1:A:347:LYS:HG3	1.95	0.66
2:B:13:LYS:HG3	2:B:14:PRO:N	2.09	0.66
2:B:275:LYS:HD2	2:B:302:GLU:HG3	1.76	0.66
2:B:195:ILE:HG13	2:B:196:GLY:H	1.60	0.66
2:B:169:GLU:N	2:B:170:PRO:HD2	2.10	0.66
1:A:232:TYR:O	1:A:242:GLN:NE2	2.21	0.65
1:A:235:HIS:HB2	1:A:238:LYS:O	1.96	0.65
2:B:67:ASP:HB2	2:B:230:MET:CG	2.26	0.65
1:A:546:GLU:HA	1:A:549:ASP:HB2	1.77	0.65
2:B:281:LYS:O	2:B:284:ARG:HD2	1.97	0.65
1:A:366:LYS:NZ	1:A:370:GLU:OE2	2.29	0.65
1:A:110:ASP:CB	1:A:219:LYS:HB3	2.26	0.65
2:B:238:LYS:NZ	2:B:351:THR:O	2.28	0.65
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.79	0.64
2:B:5:ILE:HG23	2:B:5:ILE:O	1.96	0.64
1:A:23:GLN:NE2	1:A:24:TRP:HB2	2.12	0.64
2:B:44:GLU:HG3	2:B:46:LYS:CG	2.26	0.64
1:A:253:THR:HA	1:A:291:GLU:O	1.98	0.64
1:A:283:LEU:HB2	1:A:284:ARG:NH1	2.12	0.64
1:A:550:LYS:HB3	1:A:550:LYS:HZ2	1.61	0.64
1:A:443:ASP:HB3	1:A:548:VAL:HG11	1.80	0.63
2:B:160:PHE:HD2	2:B:160:PHE:O	1.81	0.63
2:B:275:LYS:HE3	2:B:302:GLU:HA	1.79	0.63
1:A:114:ALA:HA	1:A:214:LEU:HD22	1.80	0.63
2:B:154:LYS:C	2:B:157:PRO:HD2	2.19	0.63
1:A:295:LEU:HD22	1:A:300:GLU:OE1	1.98	0.63
1:A:320:ASP:H	1:A:343:GLN:HE22	1.45	0.63
1:A:540:LYS:HA	1:A:540:LYS:CE	2.29	0.63
1:A:251:SER:HA	1:A:292:VAL:HG13	1.80	0.63
1:A:547:GLN:HA	1:A:550:LYS:NZ	2.13	0.63
2:B:363:ASN:ND2	2:B:366:LYS:HB2	2.14	0.63
1:A:49:LYS:HG2	1:A:144:TYR:CE2	2.33	0.63
2:B:183:TYR:HE1	2:B:384:GLY:O	1.82	0.63
2:B:164:MET:HE2	2:B:187:LEU:HD11	1.81	0.62
1:A:28:GLU:HG3	1:A:135:ILE:HG23	1.80	0.62
1:A:24:TRP:CZ3	1:A:59:PRO:HB2	2.34	0.62
1:A:252:TRP:O	1:A:293:ILE:N	2.32	0.62
2:B:378:GLU:O	2:B:382:ILE:HD12	1.99	0.62
1:A:317:VAL:CG2	1:A:349:LEU:HD23	2.29	0.62
1:A:545:ASN:O	1:A:549:ASP:CB	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LYS:HG3	2:B:14:PRO:CD	2.30	0.62
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.34	0.62
2:B:167:ILE:HG23	2:B:212:TRP:CG	2.34	0.62
1:A:247:PRO:HB2	1:A:252:TRP:CH2	2.34	0.62
1:A:544:GLY:C	1:A:548:VAL:HG23	2.20	0.61
1:A:198:HIS:O	1:A:202:ILE:HG12	1.99	0.61
1:A:282:LEU:HD23	1:A:282:LEU:O	2.00	0.61
1:A:265:ASN:N	1:A:265:ASN:HD22	1.98	0.61
2:B:193:LEU:HB3	2:B:197:GLN:CG	2.25	0.61
2:B:204:GLU:O	2:B:208:HIS:HB3	2.00	0.61
1:A:102:LYS:HG2	1:A:103:LYS:N	2.14	0.61
1:A:290:THR:O	1:A:290:THR:HG22	2.01	0.61
1:A:129:ALA:HA	1:A:144:TYR:O	2.00	0.60
2:B:279:LEU:N	2:B:302:GLU:OE1	2.30	0.60
2:B:170:PRO:CG	2:B:208:HIS:NE2	2.62	0.60
1:A:37:ILE:O	1:A:40:GLU:HG2	2.01	0.60
1:A:540:LYS:HA	1:A:540:LYS:HE2	1.84	0.60
2:B:391:LEU:HB3	2:B:393:ILE:HG22	1.83	0.60
1:A:548:VAL:HA	1:A:551:LEU:HD12	1.84	0.60
2:B:178:ILE:HD11	2:B:201:LYS:CD	2.27	0.60
1:A:277:ARG:NH1	1:A:334:GLN:HB3	2.16	0.60
2:B:167:ILE:HA	2:B:212:TRP:CE2	2.37	0.60
2:B:356:ARG:HH11	2:B:356:ARG:HG2	1.65	0.60
2:B:232:TYR:HE2	2:B:374:LYS:NZ	1.90	0.60
1:A:174:GLN:HG3	1:A:174:GLN:O	2.00	0.60
1:A:441:TYR:HB3	1:A:544:GLY:HA3	1.83	0.60
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.83	0.59
1:A:110:ASP:HB2	1:A:219:LYS:HB3	1.82	0.59
1:A:95:PRO:HG2	3:A:556:QO9:H22A	1.84	0.59
1:A:13:LYS:HB3	1:A:14:PRO:CD	2.30	0.59
1:A:180:ILE:HD13	1:A:189:VAL:HG13	1.84	0.59
1:A:253:THR:H	1:A:256:ASP:HB2	1.67	0.59
1:A:294:PRO:O	1:A:295:LEU:HG	2.03	0.59
2:B:329:ILE:O	2:B:392:PRO:HG3	2.03	0.59
2:B:385:LYS:HG3	2:B:385:LYS:O	2.03	0.59
1:A:148:VAL:O	1:A:150:PRO:HD3	2.03	0.59
1:A:104:LYS:HD2	1:A:192:ASP:OD1	2.03	0.59
1:A:246:LEU:HD23	1:A:246:LEU:N	2.18	0.59
1:A:303:LEU:O	1:A:307:ARG:HG3	2.03	0.59
1:A:24:TRP:CE3	1:A:59:PRO:HB2	2.37	0.59
1:A:325:LEU:HG	1:A:387:PRO:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:VAL:HG11	2:B:187:LEU:CD1	2.26	0.58
1:A:289:LEU:O	1:A:289:LEU:HD23	2.04	0.58
1:A:447:ASN:ND2	1:A:450:THR:H	2.00	0.58
2:B:350:LYS:HG3	2:B:351:THR:N	2.18	0.58
1:A:40:GLU:CG	1:A:41:MET:N	2.66	0.58
2:B:205:LEU:O	2:B:209:LEU:HB2	2.04	0.58
2:B:171:PHE:HZ	2:B:204:GLU:HB3	1.68	0.58
1:A:550:LYS:HB3	1:A:550:LYS:HZ3	1.69	0.58
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.85	0.58
2:B:323:LYS:O	2:B:385:LYS:NZ	2.37	0.57
2:B:360:ALA:HB3	2:B:363:ASN:HB3	1.86	0.57
2:B:89:GLU:OE1	2:B:94:ILE:HG12	2.04	0.57
1:A:550:LYS:O	1:A:552:VAL:HG23	2.03	0.57
2:B:356:ARG:HH11	2:B:356:ARG:CG	2.17	0.57
2:B:205:LEU:O	2:B:205:LEU:HD23	2.02	0.57
2:B:79:GLU:O	2:B:83:ARG:HG3	2.04	0.57
2:B:196:GLY:O	2:B:200:THR:HG23	2.04	0.57
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.85	0.57
2:B:67:ASP:HB2	2:B:230:MET:HG2	1.86	0.57
1:A:277:ARG:HB2	1:A:336:GLN:HE21	1.68	0.57
2:B:330:GLN:NE2	2:B:338:THR:OG1	2.37	0.57
1:A:102:LYS:NZ	1:A:236:PRO:O	2.37	0.57
2:B:360:ALA:O	2:B:367:GLN:NE2	2.37	0.57
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.87	0.57
1:A:398:TRP:CH2	1:A:411:ILE:HG13	2.39	0.56
2:B:233:GLU:O	2:B:234:LEU:HD23	2.05	0.56
2:B:344:GLU:HB2	2:B:347:LYS:HB2	1.87	0.56
2:B:182:GLN:HG3	2:B:187:LEU:CD2	2.35	0.56
2:B:353:LYS:HE3	2:B:428:GLN:HG2	1.87	0.56
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.40	0.56
2:B:195:ILE:HG13	2:B:196:GLY:N	2.21	0.56
1:A:544:GLY:O	1:A:548:VAL:CG2	2.52	0.56
1:A:78:ARG:O	1:A:82:LYS:HG3	2.06	0.56
2:B:154:LYS:HG3	2:B:184:MET:CE	2.35	0.56
1:A:506:ILE:HG21	1:A:533:LEU:HD21	1.86	0.56
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.46	0.56
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.35	0.56
1:A:278:GLN:HE21	1:A:298:GLU:HB2	1.70	0.56
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.41	0.55
1:A:253:THR:CG2	1:A:256:ASP:HB2	2.23	0.55
2:B:111:VAL:CG1	2:B:187:LEU:HD12	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLY:O	1:A:115:TYR:HB2	2.06	0.55
1:A:358:ARG:HH11	1:A:358:ARG:HG2	1.72	0.55
1:A:284:ARG:CD	1:A:358:ARG:HH22	2.19	0.55
1:A:545:ASN:O	1:A:549:ASP:CG	2.45	0.55
2:B:104:LYS:CG	2:B:192:ASP:HA	2.37	0.55
2:B:156:SER:N	2:B:157:PRO:HD2	2.21	0.55
2:B:193:LEU:CB	2:B:197:GLN:HG3	2.31	0.55
2:B:99:GLY:O	2:B:103:LYS:HG2	2.07	0.55
2:B:353:LYS:CE	2:B:428:GLN:HE21	2.19	0.55
1:A:128:THR:CG2	1:A:146:TYR:H	2.20	0.55
2:B:361:HIS:O	2:B:361:HIS:ND1	2.39	0.55
2:B:183:TYR:CE1	2:B:384:GLY:O	2.60	0.55
1:A:128:THR:CG2	1:A:146:TYR:HD2	2.20	0.55
1:A:433:PRO:HB2	2:B:290:THR:HG22	1.88	0.55
1:A:13:LYS:CB	1:A:14:PRO:HD2	2.31	0.54
1:A:451:LYS:HE2	1:A:471:ASN:HA	1.89	0.54
1:A:445:ALA:O	1:A:453:GLY:HA3	2.07	0.54
2:B:13:LYS:HE3	2:B:14:PRO:HG2	1.89	0.54
2:B:279:LEU:O	2:B:282:LEU:CD1	2.55	0.54
1:A:253:THR:N	1:A:256:ASP:HB3	2.23	0.54
2:B:314:VAL:HB	2:B:317:VAL:HG21	1.90	0.54
2:B:324:ASP:HA	2:B:385:LYS:NZ	2.22	0.54
1:A:162:SER:OG	2:B:52:PRO:HD3	2.07	0.54
1:A:186:ASP:OD2	1:A:220:LYS:HD2	2.06	0.54
1:A:542:ILE:N	1:A:546:GLU:HB2	2.22	0.54
2:B:240:THR:HG23	2:B:241:VAL:N	2.23	0.54
2:B:90:VAL:O	2:B:90:VAL:HG22	2.08	0.54
1:A:92:LEU:HD12	1:A:92:LEU:H	1.73	0.54
1:A:284:ARG:HE	1:A:358:ARG:HH22	1.54	0.54
1:A:207:GLN:HB3	1:A:211:ARG:NH2	2.23	0.53
2:B:228:LEU:HD23	2:B:228:LEU:N	2.23	0.53
1:A:156:SER:O	1:A:160:SER:HB2	2.06	0.53
2:B:169:GLU:HB3	2:B:173:LYS:NZ	2.23	0.53
1:A:105:SER:O	1:A:190:GLY:HA2	2.08	0.53
2:B:126:LYS:HA	2:B:145:GLN:OE1	2.09	0.53
1:A:296:THR:O	1:A:299:ALA:HB3	2.09	0.53
2:B:154:LYS:O	2:B:157:PRO:HD2	2.08	0.53
2:B:160:PHE:CD2	2:B:160:PHE:O	2.61	0.53
2:B:181:TYR:CG	2:B:182:GLN:N	2.77	0.53
1:A:217:PRO:O	1:A:219:LYS:N	2.41	0.53
1:A:270:ILE:HG23	1:A:271:TYR:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.53
1:A:283:LEU:CB	1:A:284:ARG:HH12	2.20	0.52
1:A:83:ARG:HG2	1:A:83:ARG:NH1	2.24	0.52
1:A:445:ALA:O	1:A:477:THR:HG21	2.08	0.52
1:A:42:GLU:OE1	1:A:49:LYS:HE2	2.09	0.52
1:A:458:VAL:CG2	2:B:286:THR:HG21	2.39	0.52
1:A:49:LYS:HG2	1:A:144:TYR:HE2	1.73	0.52
1:A:228:LEU:HD23	1:A:228:LEU:N	2.23	0.52
1:A:450:THR:HG23	1:A:452:LEU:N	2.25	0.52
2:B:205:LEU:C	2:B:205:LEU:HD23	2.30	0.52
2:B:5:ILE:CG2	2:B:5:ILE:O	2.57	0.52
1:A:541:GLY:CA	1:A:546:GLU:HG2	2.39	0.52
2:B:279:LEU:O	2:B:282:LEU:HD13	2.10	0.52
1:A:441:TYR:HB3	1:A:544:GLY:CA	2.40	0.52
1:A:78:ARG:HG2	1:A:82:LYS:HE3	1.92	0.52
2:B:240:THR:HG23	2:B:241:VAL:H	1.75	0.52
2:B:104:LYS:HG3	2:B:192:ASP:HA	1.91	0.51
1:A:112:GLY:O	1:A:116:PHE:CD2	2.63	0.51
2:B:67:ASP:HB2	2:B:230:MET:HG3	1.91	0.51
1:A:406:TRP:CD2	2:B:420:PRO:HB3	2.45	0.51
2:B:165:THR:O	2:B:169:GLU:HG3	2.10	0.51
2:B:70:LYS:HG2	2:B:71:TRP:O	2.10	0.51
2:B:399:GLU:HA	2:B:402:TRP:CD1	2.45	0.51
2:B:239:TRP:N	2:B:239:TRP:CE3	2.78	0.51
1:A:251:SER:OG	1:A:292:VAL:HG22	2.10	0.51
2:B:325:LEU:HD23	2:B:343:GLN:CG	2.41	0.51
1:A:23:GLN:NE2	1:A:24:TRP:H	2.09	0.51
2:B:195:ILE:CG1	2:B:196:GLY:N	2.73	0.51
2:B:33:ALA:O	2:B:37:ILE:HG13	2.11	0.51
1:A:299:ALA:O	1:A:302:GLU:HG2	2.11	0.51
1:A:542:ILE:CG2	2:B:283:LEU:HB3	2.36	0.50
1:A:177:ASP:OD1	1:A:177:ASP:C	2.50	0.50
1:A:424:LYS:HB2	4:A:581:HOH:O	2.10	0.50
3:A:556:QO9:HN3	3:A:556:QO9:H10A	1.76	0.50
1:A:91:GLN:NE2	1:A:92:LEU:N	2.58	0.50
2:B:167:ILE:HG23	2:B:212:TRP:CD1	2.47	0.50
2:B:209:LEU:HD23	2:B:214:LEU:HD22	1.93	0.50
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.93	0.50
1:A:366:LYS:O	1:A:370:GLU:HG3	2.11	0.50
1:A:106:VAL:HA	1:A:189:VAL:O	2.12	0.50
1:A:523:GLU:OE1	1:A:523:GLU:HA	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:GLU:N	2:B:170:PRO:CD	2.75	0.50
2:B:201:LYS:HA	2:B:201:LYS:NZ	2.27	0.50
2:B:324:ASP:HA	2:B:385:LYS:HZ1	1.77	0.50
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.47	0.50
1:A:125:ARG:O	1:A:128:THR:HB	2.12	0.49
1:A:486:LEU:HB3	1:A:524:GLN:HB3	1.94	0.49
2:B:164:MET:HE1	2:B:187:LEU:HD11	1.93	0.49
1:A:545:ASN:O	1:A:549:ASP:HB2	2.11	0.49
2:B:398:TRP:NE1	2:B:402:TRP:CD1	2.80	0.49
1:A:411:ILE:HG22	1:A:412:PRO:O	2.12	0.49
2:B:142:ILE:HG22	2:B:144:TYR:CE1	2.47	0.49
2:B:107:THR:HG23	2:B:198:HIS:HE2	1.77	0.49
1:A:541:GLY:HA2	1:A:546:GLU:CG	2.41	0.49
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.95	0.49
2:B:353:LYS:CE	2:B:428:GLN:HG2	2.42	0.49
2:B:388:LYS:CE	2:B:415:GLU:HG2	2.42	0.49
1:A:257:ILE:O	1:A:261:VAL:HG23	2.13	0.49
1:A:441:TYR:CB	1:A:544:GLY:CA	2.86	0.49
1:A:2:ILE:HD11	1:A:210:LEU:O	2.13	0.49
1:A:550:LYS:C	1:A:552:VAL:H	2.16	0.49
2:B:239:TRP:HE3	2:B:239:TRP:N	2.10	0.49
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.95	0.49
1:A:104:LYS:N	1:A:192:ASP:OD1	2.43	0.49
1:A:483:TYR:O	1:A:487:GLN:HG3	2.13	0.49
1:A:48:SER:O	1:A:144:TYR:HA	2.12	0.49
1:A:476:LYS:HG3	1:A:517:LEU:HD23	1.95	0.49
1:A:542:ILE:HG21	2:B:283:LEU:HD13	1.93	0.49
1:A:11:LYS:O	1:A:85:GLN:HB3	2.13	0.48
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.95	0.48
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.77	0.48
1:A:89:GLU:HG3	1:A:91:GLN:H	1.78	0.48
2:B:65:LYS:HG3	2:B:66:LYS:N	2.28	0.48
1:A:172:LYS:HE2	1:A:180:ILE:HB	1.94	0.48
1:A:128:THR:HG21	1:A:146:TYR:CB	2.35	0.48
1:A:181:TYR:HB2	1:A:188:TYR:HB2	1.95	0.48
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.13	0.48
1:A:460:ASN:HA	2:B:286:THR:O	2.14	0.48
1:A:541:GLY:CA	1:A:546:GLU:CG	2.91	0.48
2:B:70:LYS:HG2	2:B:71:TRP:N	2.28	0.48
2:B:284:ARG:HB3	2:B:284:ARG:HH11	1.76	0.48
1:A:102:LYS:HE3	1:A:236:PRO:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:NE	1:A:216:THR:O	2.31	0.48
2:B:12:LEU:HD12	2:B:16:MET:O	2.12	0.48
2:B:275:LYS:CD	2:B:302:GLU:HG3	2.41	0.48
1:A:210:LEU:O	1:A:210:LEU:HG	2.13	0.48
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.12	0.48
1:A:312:GLU:O	1:A:314:VAL:HG23	2.14	0.48
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.48	0.48
1:A:458:VAL:HG23	2:B:286:THR:HG21	1.95	0.48
1:A:547:GLN:HA	1:A:550:LYS:HZ3	1.79	0.48
1:A:111:VAL:O	1:A:111:VAL:CG1	2.62	0.47
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.48	0.47
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.50	0.47
1:A:111:VAL:HG21	1:A:164:MET:CE	2.44	0.47
1:A:102:LYS:CG	1:A:103:LYS:N	2.77	0.47
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.45	0.47
2:B:380:ILE:O	2:B:384:GLY:N	2.46	0.47
2:B:203:GLU:O	2:B:207:GLN:HB2	2.15	0.47
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.80	0.47
1:A:284:ARG:HD3	1:A:358:ARG:HH22	1.79	0.47
1:A:102:LYS:CE	1:A:236:PRO:O	2.63	0.47
2:B:201:LYS:HA	2:B:201:LYS:HZ3	1.79	0.47
2:B:65:LYS:HG3	2:B:66:LYS:H	1.80	0.47
1:A:277:ARG:HH11	1:A:334:GLN:HB3	1.80	0.47
2:B:115:TYR:OH	2:B:157:PRO:HA	2.15	0.47
1:A:417:VAL:O	1:A:417:VAL:HG13	2.15	0.47
2:B:209:LEU:HD23	2:B:214:LEU:CD2	2.45	0.47
2:B:263:LYS:HG3	2:B:426:TRP:CD1	2.50	0.47
2:B:227:PHE:HB3	2:B:228:LEU:HD23	1.97	0.46
2:B:96:HIS:ND1	2:B:97:PRO:HD2	2.30	0.46
1:A:68:SER:CB	1:A:70:LYS:HE3	2.30	0.46
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.97	0.46
1:A:219:LYS:O	1:A:220:LYS:C	2.50	0.46
1:A:450:THR:O	1:A:451:LYS:HB2	2.16	0.46
2:B:105:SER:O	2:B:190:GLY:HA2	2.16	0.46
2:B:335:GLY:HA2	2:B:367:GLN:OE1	2.16	0.46
1:A:180:ILE:CD1	1:A:189:VAL:HG13	2.45	0.46
1:A:77:PHE:O	1:A:78:ARG:C	2.53	0.46
2:B:122:GLU:OE2	2:B:125:ARG:CZ	2.63	0.46
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.45	0.46
1:A:113:ASP:HA	1:A:116:PHE:CD2	2.51	0.46
1:A:42:GLU:OE2	1:A:49:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:GLU:CD	2:B:71:TRP:HZ2	2.19	0.46
2:B:182:GLN:HG3	2:B:187:LEU:HD21	1.98	0.46
2:B:182:GLN:HG3	2:B:187:LEU:HD23	1.98	0.46
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.81	0.46
1:A:515:SER:C	1:A:517:LEU:N	2.70	0.46
1:A:240:THR:HG23	1:A:241:VAL:O	2.16	0.46
2:B:13:LYS:CG	2:B:14:PRO:HD2	2.45	0.46
2:B:76:ASP:OD1	2:B:78:ARG:HG3	2.16	0.46
1:A:193:LEU:HD13	1:A:197:GLN:HG2	1.98	0.45
1:A:293:ILE:CG2	1:A:294:PRO:HD2	2.45	0.45
1:A:79:GLU:OE2	1:A:83:ARG:NE	2.50	0.45
2:B:98:ALA:HB1	2:B:101:LYS:NZ	2.32	0.45
1:A:25:PRO:O	1:A:25:PRO:HG2	2.17	0.45
1:A:139:THR:HG22	1:A:140:PRO:CD	2.46	0.45
1:A:324:ASP:OD1	1:A:324:ASP:N	2.49	0.45
1:A:40:GLU:HG3	1:A:41:MET:H	1.73	0.45
2:B:376:THR:HG21	2:B:410:TRP:CE3	2.51	0.45
1:A:305:GLU:O	1:A:309:ILE:HG13	2.16	0.45
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.16	0.45
2:B:402:TRP:CH2	2:B:403:THR:HG22	2.52	0.45
1:A:111:VAL:HG22	1:A:114:ALA:HB3	1.99	0.45
2:B:242:GLN:HA	2:B:243:PRO:HD3	1.79	0.45
1:A:358:ARG:HG2	1:A:358:ARG:NH1	2.31	0.45
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.52	0.45
2:B:356:ARG:NH1	2:B:356:ARG:CG	2.79	0.45
1:A:244:ILE:CG2	1:A:263:LYS:HB3	2.47	0.45
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.32	0.45
1:A:302:GLU:HG3	1:A:303:LEU:N	2.31	0.45
1:A:308:GLU:HA	1:A:311:LYS:HE3	1.98	0.45
1:A:350:LYS:HD3	1:A:378:GLU:OE2	2.16	0.45
1:A:128:THR:HG21	1:A:146:TYR:H	1.82	0.44
1:A:223:LYS:HA	1:A:223:LYS:HD2	1.85	0.44
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.52	0.44
2:B:11:LYS:O	2:B:12:LEU:HD23	2.18	0.44
2:B:75:VAL:HB	2:B:77:PHE:CE1	2.52	0.44
2:B:30:LYS:HG2	2:B:62:ALA:HB3	2.00	0.44
2:B:44:GLU:OE1	2:B:46:LYS:HG3	2.17	0.44
2:B:98:ALA:HB1	2:B:101:LYS:HZ1	1.81	0.44
2:B:280:SER:O	2:B:283:LEU:HB2	2.18	0.44
2:B:195:ILE:O	2:B:196:GLY:C	2.56	0.44
2:B:354:TYR:CE1	2:B:356:ARG:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:PRO:HB2	2:B:423:VAL:HG22	1.98	0.44
1:A:447:ASN:HD22	1:A:450:THR:H	1.65	0.44
1:A:506:ILE:HD13	1:A:525:LEU:HD11	2.00	0.44
1:A:445:ALA:N	1:A:477:THR:OG1	2.50	0.44
1:A:550:LYS:C	1:A:552:VAL:N	2.71	0.44
1:A:249:LYS:HD3	1:A:256:ASP:OD1	2.17	0.44
1:A:508:ALA:C	1:A:509:GLN:HG3	2.38	0.44
2:B:195:ILE:HD12	2:B:196:GLY:N	2.33	0.44
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.98	0.43
1:A:544:GLY:O	1:A:548:VAL:CB	2.66	0.43
2:B:325:LEU:HD23	2:B:343:GLN:HG2	2.00	0.43
1:A:128:THR:O	1:A:128:THR:CG2	2.66	0.43
1:A:253:THR:OG1	1:A:254:VAL:N	2.50	0.43
2:B:202:ILE:O	2:B:206:ARG:HB2	2.18	0.43
1:A:252:TRP:HA	1:A:256:ASP:OD1	2.18	0.43
1:A:515:SER:C	1:A:517:LEU:H	2.21	0.43
2:B:181:TYR:HD2	2:B:188:TYR:CD1	2.36	0.43
2:B:13:LYS:HG3	2:B:14:PRO:HD2	2.00	0.43
1:A:155:GLY:O	1:A:159:ILE:HG13	2.19	0.43
2:B:282:LEU:N	2:B:282:LEU:HD12	2.20	0.43
2:B:34:LEU:HD22	2:B:73:LYS:HG3	2.01	0.43
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.18	0.43
2:B:160:PHE:O	2:B:163:SER:HB3	2.18	0.43
1:A:101:LYS:O	3:A:556:QO9:H12	2.18	0.43
1:A:63:ILE:O	1:A:63:ILE:HG23	2.19	0.43
1:A:282:LEU:CD2	1:A:282:LEU:O	2.66	0.43
1:A:301:LEU:O	1:A:304:ALA:HB3	2.19	0.43
1:A:245:VAL:C	1:A:246:LEU:HD23	2.38	0.43
2:B:170:PRO:HG3	2:B:212:TRP:NE1	2.18	0.43
2:B:376:THR:CG2	2:B:410:TRP:CZ3	3.01	0.43
2:B:191:SER:HB2	2:B:193:LEU:HG	2.00	0.42
2:B:72:ARG:HG3	2:B:73:LYS:N	2.34	0.42
1:A:344:GLU:HG3	1:A:347:LYS:HB2	2.01	0.42
2:B:180:ILE:HG12	2:B:189:VAL:HG13	2.02	0.42
2:B:108:VAL:CG1	2:B:186:ASP:HB3	2.49	0.42
1:A:161:GLN:HG2	1:A:182:GLN:NE2	2.34	0.42
2:B:353:LYS:HE3	2:B:428:GLN:NE2	2.35	0.42
2:B:388:LYS:HE2	2:B:415:GLU:HG2	2.01	0.42
1:A:50:ILE:CG1	1:A:143:ARG:HB3	2.49	0.42
1:A:168:LEU:HD13	1:A:180:ILE:HG21	2.00	0.42
1:A:546:GLU:OE1	1:A:546:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:GLN:HA	1:A:550:LYS:HZ1	1.84	0.42
2:B:156:SER:N	2:B:157:PRO:CD	2.82	0.42
2:B:178:ILE:CG2	2:B:179:VAL:N	2.82	0.42
2:B:242:GLN:H	2:B:351:THR:HG1	1.61	0.42
1:A:49:LYS:HA	1:A:143:ARG:O	2.19	0.42
2:B:168:LEU:C	2:B:170:PRO:HD2	2.39	0.42
1:A:255:ASN:HB2	1:A:289:LEU:HD21	1.98	0.42
1:A:48:SER:O	1:A:144:TYR:HD2	2.03	0.42
1:A:503:LEU:HA	1:A:503:LEU:HD12	1.78	0.42
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.55	0.41
2:B:382:ILE:HB	2:B:383:TRP:CE3	2.56	0.41
2:B:399:GLU:HA	2:B:402:TRP:HD1	1.85	0.41
1:A:207:GLN:O	1:A:211:ARG:CZ	2.69	0.41
1:A:401:TRP:CD1	1:A:402:TRP:N	2.88	0.41
2:B:118:VAL:HA	2:B:119:PRO:HD3	1.90	0.41
2:B:391:LEU:HA	2:B:392:PRO:HD3	1.78	0.41
1:A:128:THR:HG22	1:A:146:TYR:H	1.86	0.41
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.55	0.41
1:A:65:LYS:O	1:A:68:SER:HB2	2.20	0.41
1:A:89:GLU:HG2	1:A:92:LEU:HD12	2.03	0.41
2:B:115:TYR:HD1	2:B:156:SER:HG	1.62	0.41
2:B:427:TYR:O	2:B:428:GLN:OE1	2.37	0.41
2:B:154:LYS:HG3	2:B:184:MET:HE1	2.02	0.41
1:A:128:THR:CG2	1:A:146:TYR:CD2	3.02	0.41
1:A:346:PHE:O	1:A:347:LYS:HG2	2.20	0.41
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.83	0.41
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.56	0.41
2:B:77:PHE:O	2:B:78:ARG:C	2.57	0.41
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.36	0.41
2:B:104:LYS:H	2:B:104:LYS:HG2	1.70	0.41
2:B:210:LEU:HA	2:B:214:LEU:HB3	2.02	0.41
1:A:278:GLN:HA	1:A:278:GLN:OE1	2.21	0.41
1:A:283:LEU:CB	1:A:284:ARG:NH1	2.80	0.41
1:A:2:ILE:HD13	1:A:2:ILE:HA	1.79	0.41
1:A:452:LEU:HD23	1:A:470:THR:HA	2.03	0.41
1:A:541:GLY:C	1:A:546:GLU:CB	2.87	0.40
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.56	0.40
1:A:111:VAL:HG21	1:A:164:MET:HE1	2.03	0.40
2:B:13:LYS:HD2	2:B:14:PRO:HD2	2.03	0.40
2:B:161:GLN:C	2:B:163:SER:H	2.24	0.40
2:B:197:GLN:C	2:B:197:GLN:CD	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:GLU:HG2	2:B:233:GLU:H	1.51	0.40
2:B:283:LEU:HD23	2:B:283:LEU:HA	1.94	0.40
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.56	0.40
1:A:136:ASN:O	1:A:137:ASN:CB	2.67	0.40
1:A:301:LEU:O	1:A:304:ALA:N	2.54	0.40
1:A:479:LEU:HD13	1:A:518:VAL:HG22	2.03	0.40
1:A:506:ILE:CD1	1:A:525:LEU:HD11	2.51	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	551/557 (99%)	497 (90%)	51 (9%)	3 (0%)	29	52
2	B	408/428 (95%)	364 (89%)	43 (10%)	1 (0%)	47	71
All	All	959/985 (97%)	861 (90%)	94 (10%)	4 (0%)	34	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
2	B	95	PRO
1	A	294	PRO
1	A	25	PRO

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	495/497 (100%)	460 (93%)	35 (7%)	14	29
2	B	374/390 (96%)	343 (92%)	31 (8%)	11	22
All	All	869/887 (98%)	803 (92%)	66 (8%)	13	26

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

Mol	Chain	Res	Type
1	A	6	GLU
1	A	24	TRP
1	A	53	GLU
1	A	60	VAL
1	A	83	ARG
1	A	91	GLN
1	A	111	VAL
1	A	122	GLU
1	A	139	THR
1	A	174	GLN
1	A	177	ASP
1	A	186	ASP
1	A	216	THR
1	A	218	ASP
1	A	237	ASP
1	A	244	ILE
1	A	246	LEU
1	A	248	GLU
1	A	249	LYS
1	A	253	THR
1	A	265	ASN
1	A	284	ARG
1	A	291	GLU
1	A	324	ASP
1	A	358	ARG
1	A	361	HIS
1	A	366	LYS
1	A	394	GLN
1	A	431	LYS
1	A	447	ASN
1	A	463	ARG
1	A	476	LYS
1	A	512	LYS

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Mol	Chain	Res	Type
1	A	540	LYS
1	A	550	LYS
2	B	7	THR
2	B	13	LYS
2	B	48	SER
2	B	67	ASP
2	B	74	LEU
2	B	84	THR
2	B	87	PHE
2	B	122	GLU
2	B	126	LYS
2	B	160	PHE
2	B	161	GLN
2	B	171	PHE
2	B	182	GLN
2	B	201	LYS
2	B	208	HIS
2	B	209	LEU
2	B	228	LEU
2	B	230	MET
2	B	232	TYR
2	B	233	GLU
2	B	237	ASP
2	B	238	LYS
2	B	244	ILE
2	B	275	LYS
2	B	277	ARG
2	B	282	LEU
2	B	284	ARG
2	B	300	GLU
2	B	317	VAL
2	B	356	ARG
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	147	ASN
1	A	182	GLN
1	A	207	GLN
1	A	265	ASN

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Mol	Chain	Res	Type
1	A	278	GLN
1	A	315	HIS
1	A	336	GLN
1	A	343	GLN
1	A	394	GLN
1	A	428	GLN
1	A	447	ASN
1	A	475	GLN
1	A	487	GLN
1	A	547	GLN
2	B	161	GLN
2	B	197	GLN
2	B	330	GLN
2	B	336	GLN
2	B	340	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 carbohydrates 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	QO9	A	556	-	29,40,40	2.35	7 (24%)	36,68,68	1.90	6 (16%)

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	QO9	A	556	-	-	4/31/70/70	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	556	QO9	C5-C2	-6.51	1.38	1.51
3	A	556	QO9	O8-S1	5.95	1.51	1.42
3	A	556	QO9	O7-S1	5.28	1.50	1.42
3	A	556	QO9	O1-C1	4.61	1.36	1.24
3	A	556	QO9	C1-N1	3.22	1.38	1.33
3	A	556	QO9	C9-C6	2.81	1.56	1.54
3	A	556	QO9	C10-C7	2.58	1.56	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	556	QO9	C1-N1-C4	8.10	121.98	115.14
3	A	556	QO9	O4-S1-O8	3.94	113.10	108.74
3	A	556	QO9	SI1-O5-C9	-3.32	115.64	127.97
3	A	556	QO9	O8-S1-O7	-3.09	108.57	115.51
3	A	556	QO9	O4-S1-O7	2.49	111.50	108.74
3	A	556	QO9	SI2-O6-C10	-2.39	115.04	125.52

There are no chirality outliers.

All (4) torsion outliers are listed below:

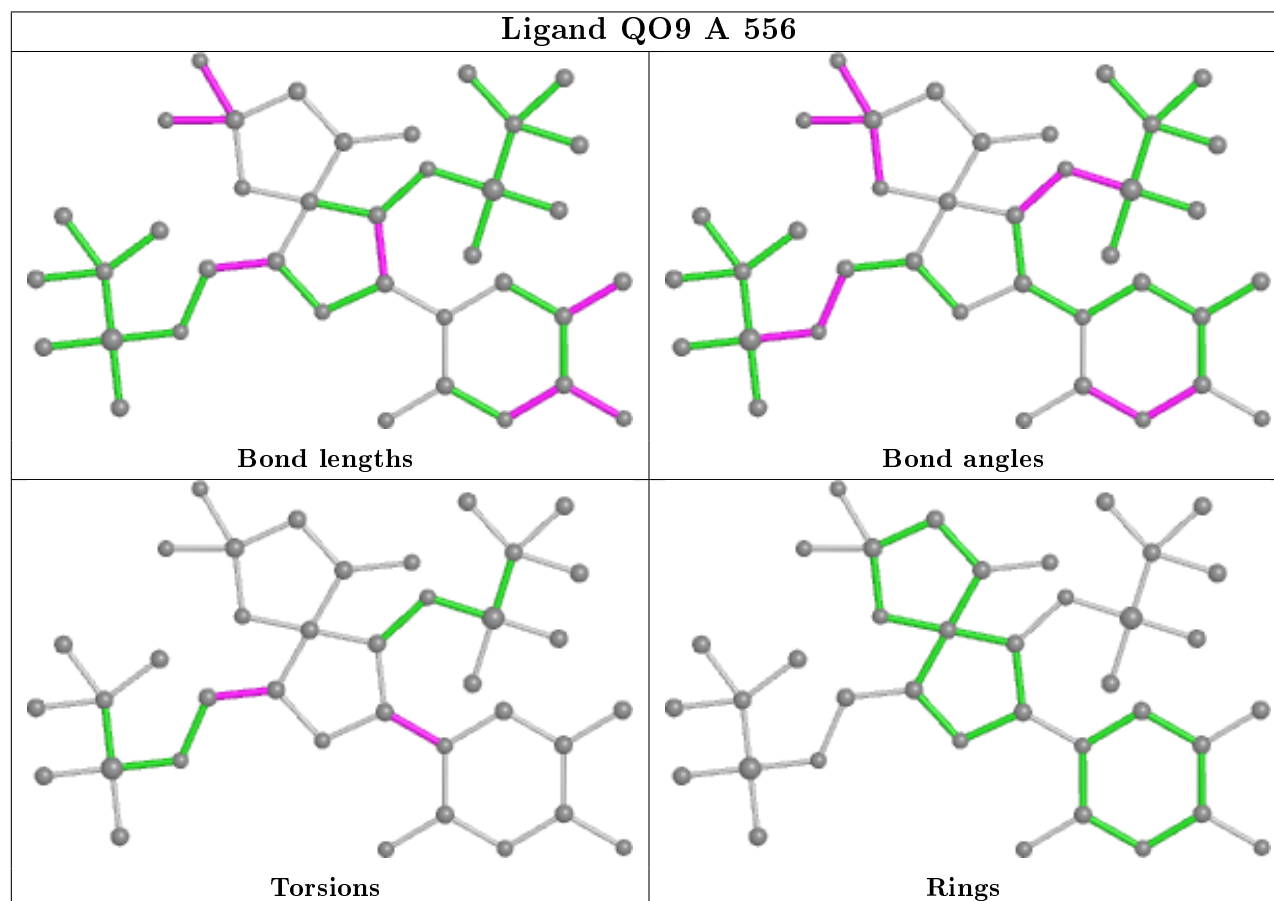
Mol	Chain	Res	Type	Atoms
3	A	556	QO9	O3-C6-N2-C3
3	A	556	QO9	C9-C6-N2-C3
3	A	556	QO9	O6-C10-C7-O3
3	A	556	QO9	O6-C10-C7-C8

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	556	QO9	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 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	553/557 (99%)	0.19	31 (5%)	24 19	47, 76, 133, 146	0
2	B	412/428 (96%)	0.33	29 (7%)	16 12	51, 81, 121, 144	0
All	All	965/985 (97%)	0.25	60 (6%)	20 15	47, 78, 126, 146	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	91	GLN	7.9
2	B	214	LEU	7.6
1	A	551	LEU	7.0
1	A	552	VAL	6.3
2	B	106	VAL	6.3
2	B	202	ILE	6.2
1	A	279	LEU	5.5
1	A	220	LYS	5.4
2	B	159	ILE	4.7
1	A	549	ASP	4.5
1	A	550	LYS	4.3
1	A	245	VAL	4.1
1	A	548	VAL	4.1
2	B	358	ARG	4.0
2	B	201	LYS	4.0
1	A	283	LEU	3.8
1	A	293	ILE	3.8
2	B	190	GLY	3.7
2	B	205	LEU	3.7
1	A	260	LEU	3.6
2	B	95	PRO	3.4
1	A	90	VAL	3.4
1	A	221	HIS	3.3
2	B	229	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	107	THR	3.2
2	B	92	LEU	3.2
2	B	227	PHE	3.1
2	B	109	LEU	3.1
1	A	247	PRO	3.1
1	A	544	GLY	3.1
1	A	246	LEU	3.0
1	A	252	TRP	3.0
1	A	219	LYS	3.0
1	A	298	GLU	2.8
1	A	66	LYS	2.8
2	B	212	TRP	2.8
2	B	16	MET	2.7
2	B	88	TRP	2.7
2	B	231	GLY	2.6
2	B	111	VAL	2.6
1	A	109	LEU	2.6
1	A	275	LYS	2.6
1	A	264	LEU	2.6
1	A	303	LEU	2.5
1	A	290	THR	2.5
1	A	288	ALA	2.5
1	A	546	GLU	2.4
2	B	209	LEU	2.4
1	A	541	GLY	2.4
2	B	149	LEU	2.4
2	B	9	PRO	2.3
2	B	67	ASP	2.3
2	B	90	VAL	2.3
1	A	115	TYR	2.3
1	A	84	THR	2.2
2	B	89	GLU	2.2
2	B	168	LEU	2.2
2	B	153	TRP	2.2
2	B	232	TYR	2.1
1	A	278	GLN	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

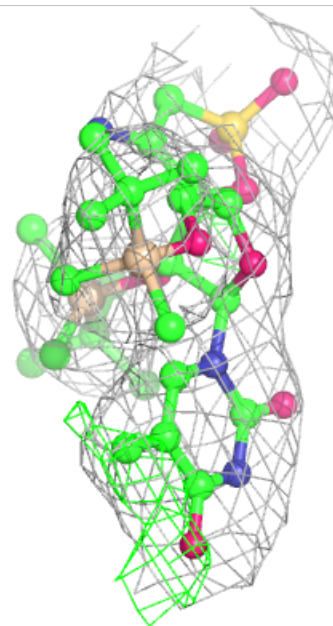
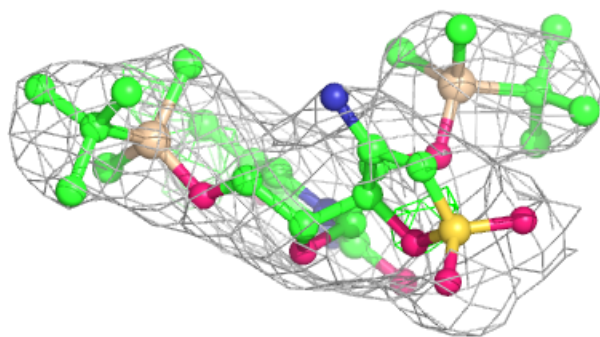
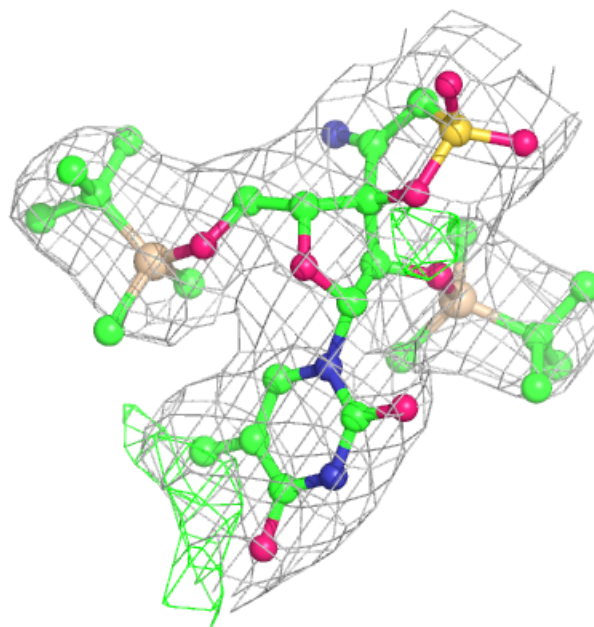
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	QO9	A	556	38/38	0.96	0.20	50,72,79,84	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 QO9 A 556:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.