Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 04:23 AM EDT

PDB ID	:	3MEG
Title	:	HIV-1 K103N Reverse Transcriptase in Complex with TMC278
Authors	:	Lansdon, E.B.
Deposited on	:	2010-03-31
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 (i) 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 (i)) were used in the production of this report:

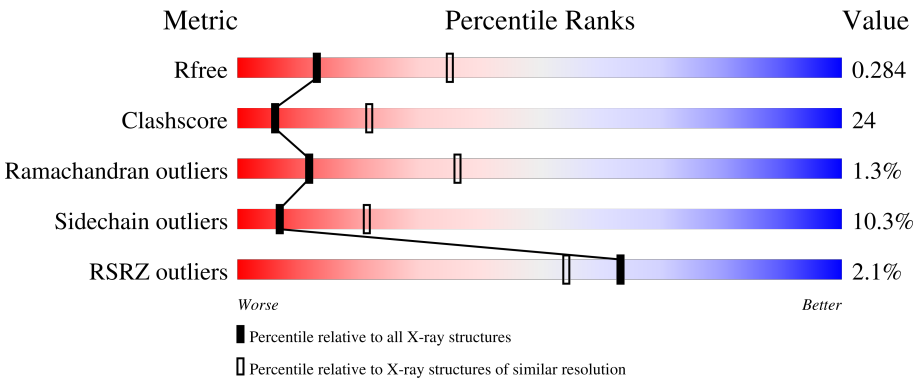
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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))
R_{free}	130704	3140 (2.80-2.80)
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 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	560	2% 51% 42% 6% •
2	B	440	2% 50% 36% 5% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7903 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 p66 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	552	4501	2909	751	833	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P04585

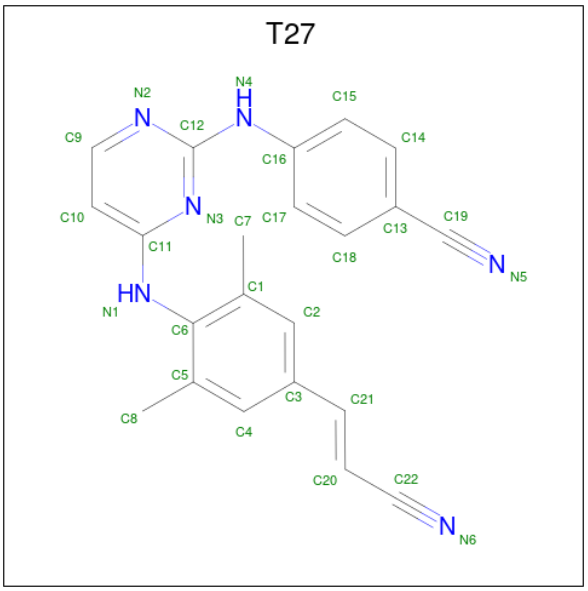
- Molecule 2 is a protein called p51 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	404	3333	2169	549	609	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

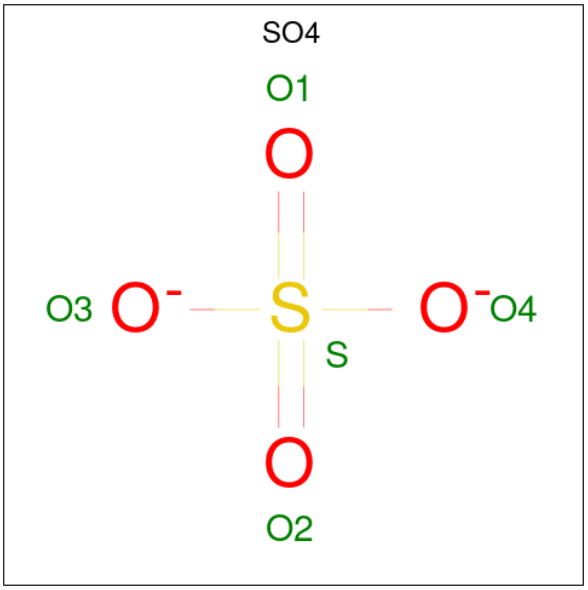
Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	engineered mutation	UNP P04585

- Molecule 3 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
			Total	C	N		
3	A	1	28	22	6	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	A	1	5	4	1	0	0
			Total	O	S		
4	B	1	5	4	1	0	0

- Molecule 5 is water.

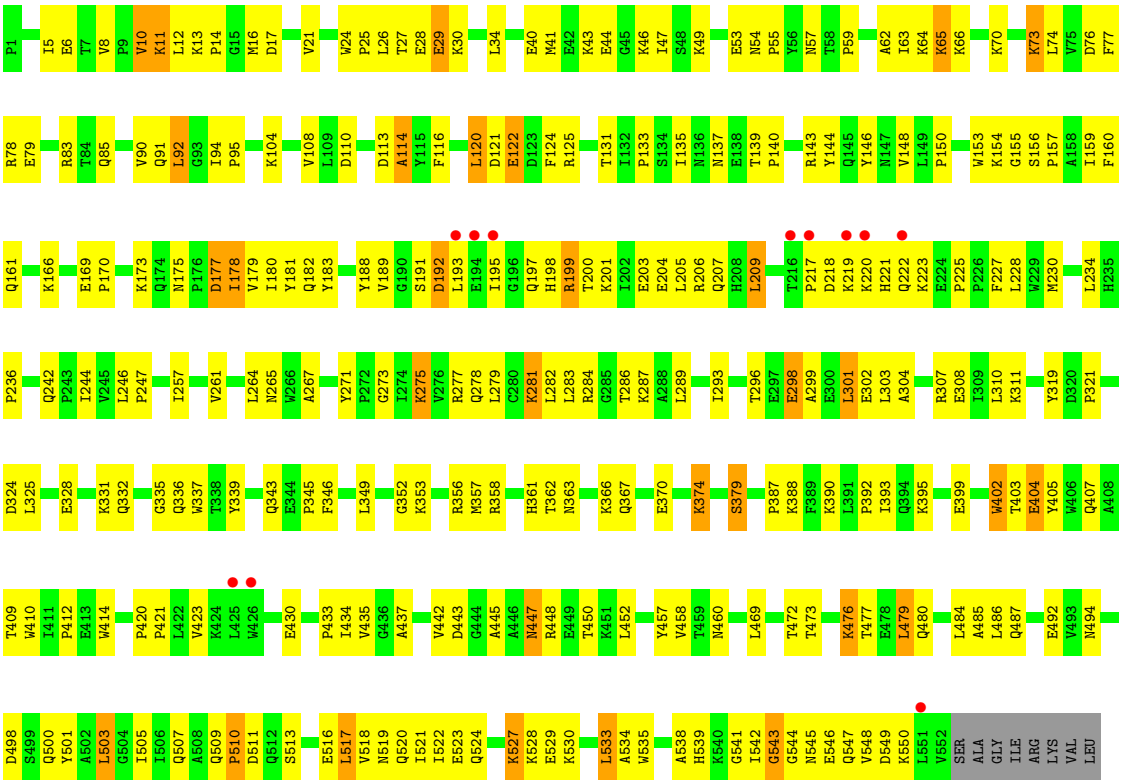
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	8	8	8	0	0
			Total	O		
5	B	8	8	8	0	0

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.

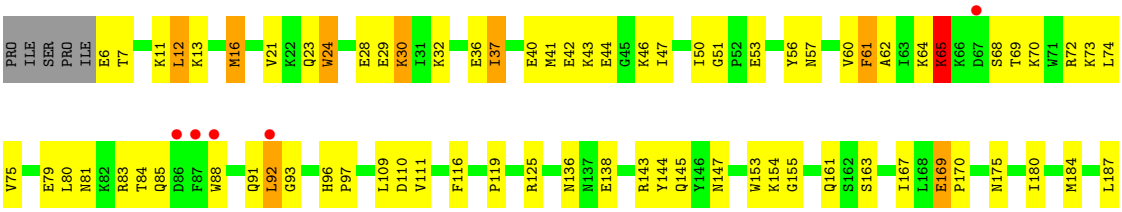
- Molecule 1: p66 Reverse transcriptase

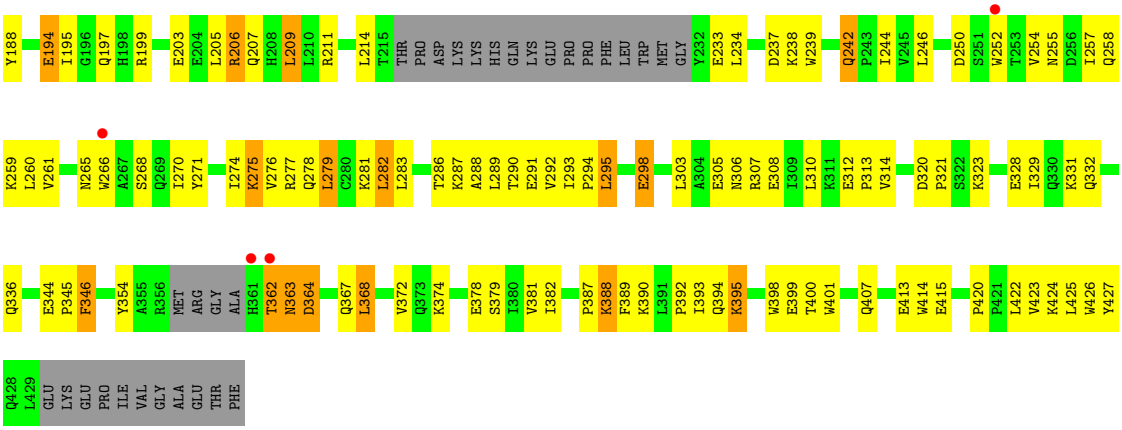
Chain A:



- Molecule 2: p51 Reverse transcriptase

Chain B:




Y188 E194 I195 G196 Q197 H198 R199 E203 E204 L205 R206 Q207 H208 L209 L210 R211 L214 T215 THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET GLY Y232 E233 L234 D237 K238 W239 Q242 P243 I244 V245 L246 D250 S251 W252 T253 V254 N255 D256 I257 Q258
K259 L260 V261 N265 W266 A267 S268 Q269 I270 Y271 I274 K275 V276 R277 Q278 L279 C280 K281 L282 L283 T286 K287 A288 L289 T290 E291 V292 I293 P294 L295 E298 L303 A304 E305 N306 R307 E308 I309 L310 K311 E312 P313 V314 D320 P321 S322 K323 E328 I329 Q330 K331 Q332
Q336 E344 P345 F346 Y354 A355 R356 MET ARG GLY ALA H361 T362 N363 D364 Q367 L368 V372 Q373 K374 E378 S379 I380 V381 I382 P387 K388 F389 K390 L391 P392 I393 Q394 K395 W398 E399 T400 W401 Q407 E413 W414 E415 P420 P421 L422 V423 K424 L425 W426 Y427
Q428 L429 GLU LYS GLU PRO ILE VAL GLY ALA GLU THR PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.58Å 154.91Å 153.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.80 47.33 – 2.79	Depositor EDS
% Data completeness (in resolution range)	85.9 (29.94-2.80) 85.7 (47.33-2.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 2.81Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.229 , 0.289 0.219 , 0.284	Depositor DCC
R_{free} test set	1498 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7903	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, T27

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	0.40	0/4618	0.55	0/6276
2	B	0.41	0/3426	0.56	0/4658
All	All	0.41	0/8044	0.55	0/10934

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	362	THR	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	4501	0	4546	229	0
2	B	3333	0	3345	176	0
3	A	28	0	18	5	0
4	A	20	0	0	0	0
4	B	5	0	0	0	0
5	A	8	0	0	0	0
5	B	8	0	0	0	0
All	All	7903	0	7909	386	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 24.

All (386) 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:199:ARG:HG2	1:A:199:ARG:HH11	1.20	1.01
2:B:13:LYS:HE3	2:B:85:GLN:HB3	1.51	0.91
2:B:362:THR:CG2	2:B:363:ASN:H	1.86	0.89
1:A:199:ARG:HG2	1:A:199:ARG:NH1	1.85	0.88
1:A:108:VAL:HG22	1:A:188:TYR:HD2	1.41	0.86
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.57	0.86
1:A:178:ILE:HD12	1:A:179:VAL:N	1.91	0.85
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.75	0.83
1:A:191:SER:HB3	1:A:198:HIS:ND1	1.94	0.82
2:B:362:THR:HG23	2:B:363:ASN:H	1.46	0.79
2:B:332:GLN:HB2	2:B:336:GLN:HB2	1.65	0.79
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.26	0.79
2:B:50:ILE:HG21	2:B:145:GLN:HG3	1.66	0.78
2:B:92:LEU:HD13	2:B:93:GLY:H	1.47	0.78
1:A:65:LYS:HE2	1:A:66:LYS:NZ	1.98	0.77
1:A:542:ILE:HG23	2:B:283:LEU:HD23	1.66	0.76
2:B:362:THR:CG2	2:B:363:ASN:N	2.45	0.76
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.51	0.76
1:A:223:LYS:HE2	1:A:223:LYS:HA	1.68	0.75
1:A:108:VAL:HG22	1:A:188:TYR:CD2	2.21	0.75
1:A:298:GLU:H	1:A:298:GLU:CD	1.90	0.74
1:A:458:VAL:HG23	1:A:548:VAL:HB	1.70	0.73
1:A:199:ARG:HH11	1:A:199:ARG:CG	1.98	0.73
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.69	0.73
2:B:46:LYS:HD3	2:B:116:PHE:CD2	2.25	0.72
1:A:278:GLN:HG3	1:A:298:GLU:HB2	1.71	0.72
1:A:94:ILE:HG23	1:A:95:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD12	1:A:535:TRP:HB2	1.70	0.71
1:A:358:ARG:NH1	2:B:394:GLN:HG3	2.06	0.71
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.26	0.71
1:A:28:GLU:HG3	1:A:135:ILE:HG23	1.71	0.71
2:B:65:LYS:O	2:B:407:GLN:HG2	1.91	0.70
2:B:244:ILE:HD12	2:B:244:ILE:H	1.56	0.70
1:A:450:THR:CG2	1:A:452:LEU:HB2	2.20	0.70
2:B:209:LEU:HB3	2:B:214:LEU:HB3	1.73	0.70
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.74	0.70
2:B:206:ARG:HH11	2:B:206:ARG:HB2	1.57	0.70
1:A:178:ILE:HD12	1:A:179:VAL:H	1.56	0.69
2:B:395:LYS:HD3	2:B:399:GLU:OE1	1.92	0.69
1:A:445:ALA:O	1:A:477:THR:HG21	1.93	0.69
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.74	0.69
2:B:354:TYR:CD2	2:B:374:LYS:HD3	2.28	0.69
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.74	0.68
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.29	0.68
1:A:301:LEU:O	1:A:304:ALA:HB3	1.93	0.68
1:A:65:LYS:HE2	1:A:66:LYS:HZ2	1.59	0.68
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.76	0.68
2:B:378:GLU:O	2:B:382:ILE:HG13	1.94	0.68
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.75	0.67
1:A:545:ASN:O	1:A:549:ASP:HB2	1.93	0.67
2:B:345:PRO:O	2:B:346:PHE:HB2	1.94	0.67
1:A:296:THR:HB	1:A:298:GLU:OE2	1.94	0.67
2:B:244:ILE:HD12	2:B:244:ILE:N	2.09	0.67
1:A:79:GLU:O	1:A:83:ARG:HG3	1.95	0.66
1:A:175:ASN:HB3	1:A:178:ILE:CG2	2.25	0.66
2:B:50:ILE:HG21	2:B:145:GLN:CG	2.25	0.66
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.78	0.65
2:B:154:LYS:HG2	2:B:184:MET:SD	2.36	0.65
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.77	0.64
2:B:194:GLU:HG3	2:B:197:GLN:HG3	1.78	0.64
1:A:11:LYS:HE3	1:A:11:LYS:HA	1.78	0.64
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.33	0.64
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.32	0.64
2:B:154:LYS:HE3	2:B:184:MET:SD	2.38	0.64
1:A:281:LYS:HG2	1:A:284:ARG:NH2	2.12	0.64
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.28	0.63
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.81	0.63
2:B:65:LYS:H	2:B:65:LYS:HD2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:TYR:O	2:B:274:ILE:HG12	1.99	0.62
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.15	0.62
1:A:27:THR:OG1	1:A:30:LYS:HG3	1.99	0.62
1:A:73:LYS:HE3	1:A:146:TYR:OH	2.00	0.62
1:A:191:SER:HB3	1:A:198:HIS:CE1	2.35	0.61
2:B:50:ILE:HD13	2:B:145:GLN:HG3	1.82	0.61
1:A:91:GLN:HG3	1:A:91:GLN:O	2.00	0.61
1:A:139:THR:HB	1:A:140:PRO:HD2	1.81	0.61
1:A:435:VAL:HA	2:B:290:THR:HG21	1.82	0.61
2:B:362:THR:HG22	2:B:363:ASN:H	1.63	0.61
1:A:175:ASN:HB3	1:A:178:ILE:HG23	1.83	0.60
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.29	0.60
1:A:450:THR:HG22	1:A:452:LEU:HB2	1.84	0.60
2:B:203:GLU:OE2	2:B:206:ARG:NH1	2.35	0.60
2:B:362:THR:HG22	2:B:363:ASN:N	2.15	0.60
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.37	0.60
2:B:65:LYS:HG2	2:B:68:SER:HB3	1.82	0.60
2:B:329:ILE:O	2:B:392:PRO:HG3	2.02	0.60
1:A:287:LYS:HD3	1:A:293:ILE:HD11	1.84	0.59
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.01	0.59
1:A:392:PRO:O	1:A:423:VAL:HG12	2.03	0.59
1:A:197:GLN:O	1:A:200:THR:HB	2.02	0.59
1:A:420:PRO:HA	1:A:421:PRO:C	2.23	0.59
1:A:65:LYS:HG2	1:A:66:LYS:HD2	1.85	0.58
2:B:295:LEU:HD13	2:B:295:LEU:N	2.19	0.58
1:A:139:THR:HB	1:A:140:PRO:CD	2.33	0.58
2:B:79:GLU:O	2:B:83:ARG:HG3	2.03	0.58
2:B:362:THR:HG23	2:B:363:ASN:N	2.15	0.58
2:B:388:LYS:HG2	2:B:413:GLU:HB2	1.85	0.58
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.18	0.58
2:B:194:GLU:CG	2:B:197:GLN:HG3	2.32	0.58
1:A:65:LYS:HE2	1:A:66:LYS:HZ3	1.69	0.58
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.18	0.58
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.18	0.58
2:B:295:LEU:HD22	2:B:295:LEU:H	1.68	0.58
1:A:195:ILE:CG2	1:A:199:ARG:HH21	2.16	0.58
2:B:254:VAL:O	2:B:258:GLN:HG3	2.04	0.58
1:A:275:LYS:HG3	1:A:332:GLN:HE21	1.69	0.58
2:B:110:ASP:O	2:B:214:LEU:HD21	2.04	0.57
2:B:163:SER:O	2:B:167:ILE:HG13	2.03	0.57
2:B:279:LEU:O	2:B:282:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:HG3	1:A:135:ILE:CG2	2.34	0.57
1:A:435:VAL:CA	2:B:290:THR:HG21	2.34	0.57
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.39	0.57
2:B:88:TRP:CZ2	2:B:154:LYS:HD2	2.38	0.57
2:B:294:PRO:C	2:B:295:LEU:HD13	2.24	0.57
1:A:177:ASP:OD2	1:A:177:ASP:N	2.37	0.57
1:A:282:LEU:H	1:A:282:LEU:HD22	1.70	0.57
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.66	0.57
1:A:435:VAL:N	2:B:290:THR:HG21	2.20	0.57
2:B:354:TYR:HB2	2:B:374:LYS:HE2	1.87	0.57
1:A:308:GLU:OE2	1:A:311:LYS:HD2	2.05	0.57
1:A:516:GLU:O	1:A:520:GLN:HG3	2.05	0.57
2:B:96:HIS:HE1	2:B:381:VAL:O	1.86	0.57
1:A:518:VAL:O	1:A:522:ILE:HG13	2.04	0.56
2:B:206:ARG:HH11	2:B:206:ARG:CB	2.17	0.56
2:B:195:ILE:O	2:B:199:ARG:HG3	2.04	0.56
2:B:246:LEU:HB2	2:B:307:ARG:HH11	1.69	0.56
2:B:81:ASN:ND2	2:B:154:LYS:HG3	2.21	0.56
2:B:331:LYS:O	2:B:424:LYS:HE3	2.04	0.56
1:A:244:ILE:HG13	1:A:244:ILE:O	2.04	0.56
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.87	0.56
2:B:291:GLU:O	2:B:293:ILE:HG23	2.05	0.56
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.88	0.56
2:B:85:GLN:HA	2:B:88:TRP:CD1	2.39	0.56
1:A:74:LEU:N	1:A:74:LEU:HD12	2.21	0.56
1:A:509:GLN:N	1:A:510:PRO:HD3	2.21	0.56
2:B:6:GLU:OE1	2:B:6:GLU:HA	2.06	0.56
2:B:242:GLN:HE21	2:B:242:GLN:C	2.09	0.56
1:A:10:VAL:HG22	1:A:124:PHE:CD1	2.42	0.55
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.41	0.55
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.88	0.55
1:A:541:GLY:HA2	1:A:546:GLU:CG	2.37	0.55
2:B:320:ASP:OD2	2:B:323:LYS:HD2	2.07	0.55
1:A:125:ARG:HG2	1:A:146:TYR:O	2.06	0.55
1:A:116:PHE:O	1:A:148:VAL:HG11	2.06	0.55
1:A:430:GLU:OE2	1:A:530:LYS:HG2	2.06	0.55
1:A:192:ASP:C	1:A:193:LEU:HD22	2.26	0.55
1:A:366:LYS:O	1:A:370:GLU:HG3	2.07	0.55
1:A:500:GLN:HG3	2:B:422:LEU:HD23	1.89	0.55
1:A:85:GLN:O	1:A:154:LYS:NZ	2.40	0.54
1:A:179:VAL:HG11	3:A:561:T27:C11	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:OE2	1:A:219:LYS:HE3	2.06	0.54
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.90	0.54
1:A:41:MET:HE3	1:A:47:ILE:HD13	1.90	0.54
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.89	0.54
3:A:561:T27:H15	3:A:561:T27:N3	2.22	0.54
1:A:434:ILE:HD12	1:A:494:ASN:OD1	2.07	0.54
2:B:47:ILE:HD12	2:B:144:TYR:CG	2.43	0.54
2:B:395:LYS:O	2:B:399:GLU:HG3	2.07	0.54
1:A:5:ILE:HG12	1:A:6:GLU:O	2.08	0.54
2:B:237:ASP:C	2:B:239:TRP:H	2.12	0.54
1:A:8:VAL:HB	1:A:159:ILE:HD12	1.90	0.53
1:A:273:GLY:HA2	1:A:332:GLN:HE22	1.73	0.53
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.43	0.53
1:A:435:VAL:HG22	2:B:290:THR:HB	1.91	0.53
2:B:308:GLU:O	2:B:312:GLU:HG2	2.07	0.53
1:A:175:ASN:OD1	1:A:201:LYS:HE2	2.09	0.53
1:A:279:LEU:O	1:A:282:LEU:HD23	2.09	0.53
2:B:279:LEU:C	2:B:281:LYS:H	2.12	0.53
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.44	0.53
1:A:12:LEU:HD22	1:A:12:LEU:H	1.73	0.52
1:A:179:VAL:HG11	3:A:561:T27:C10	2.39	0.52
2:B:37:ILE:O	2:B:41:MET:HG3	2.09	0.52
2:B:362:THR:HG21	2:B:367:GLN:OE1	2.10	0.52
1:A:547:GLN:O	1:A:550:LYS:HB3	2.09	0.52
2:B:43:LYS:O	2:B:43:LYS:HG3	2.09	0.52
2:B:244:ILE:H	2:B:244:ILE:CD1	2.22	0.52
2:B:287:LYS:HE2	2:B:291:GLU:OE2	2.08	0.52
1:A:362:THR:HG22	1:A:366:LYS:HE2	1.92	0.52
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.40	0.52
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.91	0.52
2:B:44:GLU:OE1	2:B:46:LYS:NZ	2.39	0.52
2:B:275:LYS:HZ3	2:B:277:ARG:HG2	1.75	0.52
2:B:277:ARG:HG3	2:B:278:GLN:N	2.25	0.52
1:A:324:ASP:OD1	1:A:388:LYS:HE2	2.10	0.51
1:A:513:SER:O	1:A:519:ASN:ND2	2.43	0.51
1:A:548:VAL:O	1:A:548:VAL:HG22	2.10	0.51
1:A:178:ILE:HD11	1:A:189:VAL:HG13	1.92	0.51
1:A:191:SER:OG	1:A:193:LEU:HD23	2.11	0.51
2:B:61:PHE:N	2:B:61:PHE:CD1	2.78	0.51
2:B:266:TRP:HZ2	2:B:427:TYR:CZ	2.28	0.51
1:A:110:ASP:O	1:A:217:PRO:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:HIS:HB2	1:A:222:GLN:HB3	1.93	0.51
1:A:257:ILE:O	1:A:261:VAL:HG23	2.11	0.51
1:A:402:TRP:CD1	2:B:331:LYS:NZ	2.77	0.51
2:B:306:ASN:O	2:B:310:LEU:HD22	2.11	0.51
1:A:155:GLY:O	1:A:159:ILE:HG12	2.11	0.51
2:B:354:TYR:HD2	2:B:374:LYS:HD3	1.71	0.51
2:B:92:LEU:HD13	2:B:93:GLY:N	2.20	0.51
1:A:447:ASN:C	1:A:447:ASN:HD22	2.13	0.50
1:A:399:GLU:O	1:A:403:THR:HG23	2.11	0.50
2:B:12:LEU:HD23	2:B:84:THR:HG22	1.93	0.50
1:A:542:ILE:HG22	1:A:543:GLY:N	2.26	0.50
2:B:80:LEU:HD23	2:B:84:THR:HG23	1.93	0.50
1:A:275:LYS:HD2	1:A:332:GLN:NE2	2.27	0.50
2:B:266:TRP:CD1	2:B:346:PHE:HE1	2.30	0.50
1:A:41:MET:CE	1:A:47:ILE:HD13	2.41	0.50
1:A:271:TYR:CD1	1:A:310:LEU:HD23	2.47	0.50
2:B:293:ILE:O	2:B:293:ILE:HG13	2.12	0.50
2:B:362:THR:CG2	2:B:367:GLN:OE1	2.59	0.50
2:B:36:GLU:O	2:B:37:ILE:C	2.50	0.49
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.94	0.49
1:A:447:ASN:C	1:A:447:ASN:ND2	2.65	0.49
1:A:324:ASP:CG	1:A:388:LYS:HE2	2.32	0.49
2:B:214:LEU:HD13	2:B:214:LEU:C	2.32	0.49
2:B:246:LEU:HD23	2:B:246:LEU:N	2.27	0.49
2:B:393:ILE:HG12	2:B:394:GLN:N	2.27	0.49
1:A:460:ASN:HA	2:B:286:THR:O	2.13	0.49
1:A:11:LYS:HG3	1:A:12:LEU:N	2.28	0.49
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.94	0.49
2:B:206:ARG:NH1	2:B:206:ARG:CB	2.76	0.49
2:B:274:ILE:HG23	2:B:306:ASN:OD1	2.13	0.49
1:A:236:PRO:HA	3:A:561:T27:H18	1.93	0.49
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.47	0.49
2:B:80:LEU:HD23	2:B:80:LEU:O	2.12	0.49
1:A:345:PRO:HA	1:A:346:PHE:HA	1.50	0.49
1:A:450:THR:HG21	1:A:452:LEU:HB2	1.94	0.49
2:B:271:TYR:CE1	2:B:314:VAL:HG22	2.48	0.49
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.95	0.48
2:B:74:LEU:HD12	2:B:75:VAL:N	2.27	0.48
2:B:257:ILE:O	2:B:261:VAL:HG23	2.12	0.48
2:B:16:MET:HE2	2:B:16:MET:HB3	1.80	0.48
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:GLU:H	2:B:197:GLN:HE21	1.61	0.48
2:B:207:GLN:O	2:B:211:ARG:HD3	2.13	0.48
1:A:307:ARG:O	1:A:311:LYS:HG3	2.14	0.48
1:A:447:ASN:HD22	1:A:448:ARG:N	2.11	0.48
1:A:542:ILE:HG23	2:B:283:LEU:CD2	2.42	0.48
1:A:544:GLY:O	1:A:548:VAL:HG12	2.14	0.48
2:B:21:VAL:O	2:B:57:ASN:HB3	2.14	0.48
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.43	0.48
2:B:298:GLU:HA	2:B:298:GLU:OE2	2.13	0.48
1:A:218:ASP:C	1:A:220:LYS:H	2.16	0.47
2:B:279:LEU:C	2:B:281:LYS:N	2.66	0.47
1:A:527:LYS:NZ	1:A:528:LYS:HE2	2.29	0.47
1:A:542:ILE:O	1:A:543:GLY:C	2.53	0.47
1:A:410:TRP:CE2	2:B:363:ASN:ND2	2.82	0.47
2:B:72:ARG:HG2	2:B:73:LYS:O	2.15	0.47
1:A:92:LEU:O	1:A:92:LEU:HD22	2.14	0.47
1:A:146:TYR:CG	1:A:150:PRO:HG3	2.50	0.47
1:A:195:ILE:HG23	1:A:199:ARG:HE	1.79	0.47
2:B:354:TYR:HD2	2:B:374:LYS:CD	2.27	0.47
2:B:388:LYS:HE2	2:B:415:GLU:HB3	1.97	0.47
1:A:486:LEU:CB	1:A:524:GLN:HG2	2.43	0.47
1:A:542:ILE:HB	1:A:545:ASN:CB	2.45	0.47
1:A:46:LYS:HD2	1:A:116:PHE:HB3	1.96	0.47
1:A:473:THR:H	1:A:476:LYS:HD3	1.79	0.47
1:A:122:GLU:OE1	1:A:122:GLU:HA	2.15	0.47
1:A:29:GLU:HG2	1:A:30:LYS:N	2.29	0.47
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.48	0.47
1:A:206:ARG:HH12	1:A:218:ASP:HA	1.78	0.47
1:A:281:LYS:HG2	1:A:284:ARG:CZ	2.45	0.46
1:A:404:GLU:O	1:A:404:GLU:HG2	2.13	0.46
2:B:328:GLU:HG3	2:B:390:LYS:HB2	1.96	0.46
2:B:275:LYS:HE2	2:B:276:VAL:H	1.80	0.46
1:A:153:TRP:CG	1:A:154:LYS:N	2.83	0.46
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.30	0.46
2:B:244:ILE:HG12	2:B:266:TRP:CZ3	2.50	0.46
2:B:275:LYS:NZ	2:B:277:ARG:HG2	2.31	0.46
1:A:193:LEU:HD22	1:A:193:LEU:N	2.31	0.46
1:A:374:LYS:HE3	1:A:374:LYS:HB3	1.57	0.46
2:B:30:LYS:HG3	2:B:62:ALA:HB3	1.98	0.46
1:A:527:LYS:HD3	1:A:528:LYS:HE2	1.97	0.46
2:B:295:LEU:N	2:B:295:LEU:HD22	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:NH2	1:A:358:ARG:HD2	2.31	0.46
1:A:542:ILE:HB	1:A:545:ASN:HB2	1.97	0.45
1:A:379:SER:OG	1:A:387:PRO:HG3	2.16	0.45
1:A:409:THR:O	2:B:364:ASP:HB2	2.15	0.45
2:B:303:LEU:HD22	2:B:307:ARG:NH2	2.30	0.45
1:A:543:GLY:H	2:B:283:LEU:HB3	1.80	0.45
2:B:195:ILE:HD11	2:B:233:GLU:OE1	2.16	0.45
1:A:11:LYS:HG3	1:A:12:LEU:O	2.16	0.45
1:A:286:THR:HG23	1:A:286:THR:O	2.16	0.45
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.44	0.45
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.98	0.45
2:B:400:THR:HB	2:B:401:TRP:CD1	2.52	0.45
1:A:175:ASN:O	1:A:178:ILE:HG23	2.16	0.45
1:A:225:PRO:HB3	1:A:227:PHE:CE2	2.51	0.45
1:A:538:ALA:HA	1:A:545:ASN:HD21	1.81	0.45
1:A:12:LEU:HD22	1:A:12:LEU:N	2.31	0.45
1:A:331:LYS:HB3	1:A:421:PRO:HG2	1.99	0.45
2:B:73:LYS:HZ3	2:B:73:LYS:HG3	1.53	0.45
2:B:180:ILE:HA	2:B:188:TYR:O	2.17	0.45
1:A:221:HIS:HA	1:A:222:GLN:HA	1.68	0.45
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.99	0.45
1:A:228:LEU:HD12	1:A:242:GLN:OE1	2.17	0.45
2:B:368:LEU:O	2:B:372:VAL:HG23	2.16	0.45
2:B:23:GLN:HE22	2:B:60:VAL:H	1.64	0.45
2:B:88:TRP:CH2	2:B:154:LYS:HD2	2.52	0.45
1:A:24:TRP:CD2	1:A:25:PRO:HD2	2.51	0.44
1:A:402:TRP:CG	1:A:403:THR:N	2.84	0.44
2:B:96:HIS:CE1	2:B:381:VAL:O	2.69	0.44
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.52	0.44
1:A:108:VAL:HG23	1:A:227:PHE:CE1	2.52	0.44
2:B:37:ILE:HG21	2:B:73:LYS:HB2	1.98	0.44
2:B:64:LYS:HE2	2:B:64:LYS:HB3	1.73	0.44
1:A:358:ARG:HH12	2:B:394:GLN:HG3	1.78	0.44
2:B:65:LYS:O	2:B:407:GLN:CG	2.62	0.44
2:B:47:ILE:O	2:B:47:ILE:HG13	2.18	0.44
1:A:223:LYS:HA	1:A:223:LYS:CE	2.39	0.44
2:B:244:ILE:N	2:B:244:ILE:CD1	2.78	0.44
2:B:237:ASP:C	2:B:239:TRP:N	2.71	0.44
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.00	0.44
1:A:195:ILE:CG2	1:A:199:ARG:HE	2.31	0.44
1:A:227:PHE:HB3	3:A:561:T27:N6	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.99	0.44
1:A:234:LEU:N	1:A:234:LEU:HD22	2.33	0.43
1:A:156:SER:N	1:A:157:PRO:HD2	2.33	0.43
1:A:279:LEU:HA	1:A:282:LEU:CD2	2.48	0.43
1:A:457:TYR:HA	1:A:548:VAL:HG21	1.99	0.43
2:B:13:LYS:CE	2:B:85:GLN:HB3	2.35	0.43
2:B:320:ASP:HA	2:B:321:PRO:HD2	1.80	0.43
2:B:56:TYR:O	2:B:143:ARG:NH2	2.51	0.43
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.53	0.43
1:A:63:ILE:HG22	1:A:74:LEU:CD1	2.49	0.43
1:A:5:ILE:CG1	1:A:6:GLU:N	2.82	0.43
1:A:54:ASN:O	1:A:143:ARG:NH2	2.52	0.43
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.80	0.43
2:B:268:SER:C	2:B:270:ILE:H	2.22	0.43
2:B:422:LEU:O	2:B:425:LEU:HG	2.19	0.43
2:B:51:GLY:HA3	2:B:53:GLU:OE2	2.19	0.43
2:B:379:SER:OG	2:B:387:PRO:HD3	2.19	0.43
1:A:183:TYR:OH	1:A:230:MET:HE1	2.19	0.43
1:A:457:TYR:CD1	1:A:457:TYR:C	2.92	0.43
2:B:420:PRO:HG2	2:B:423:VAL:CG2	2.49	0.43
1:A:120:LEU:HD22	1:A:121:ASP:H	1.84	0.42
1:A:501:TYR:O	1:A:505:ILE:HG13	2.19	0.42
2:B:252:TRP:HD1	2:B:295:LEU:HD12	1.84	0.42
2:B:69:THR:O	2:B:70:LYS:HG3	2.19	0.42
1:A:484:LEU:HD23	1:A:487:GLN:HE21	1.84	0.42
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.90	0.42
2:B:169:GLU:HB3	2:B:170:PRO:HD3	2.01	0.42
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.45	0.42
2:B:237:ASP:O	2:B:239:TRP:N	2.52	0.42
1:A:26:LEU:HD12	1:A:133:PRO:HG3	2.01	0.42
2:B:28:GLU:HG2	2:B:32:LYS:HE2	2.01	0.42
2:B:42:GLU:C	2:B:44:GLU:H	2.23	0.42
1:A:228:LEU:N	1:A:228:LEU:HD22	2.34	0.42
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.39	0.42
1:A:520:GLN:C	1:A:522:ILE:N	2.73	0.42
1:A:472:THR:HB	1:A:476:LYS:HB2	2.01	0.42
1:A:529:GLU:O	1:A:530:LYS:HG3	2.20	0.41
2:B:136:ASN:HB3	2:B:138:GLU:HG3	2.02	0.41
1:A:218:ASP:HB3	1:A:221:HIS:CE1	2.54	0.41
1:A:533:LEU:HD22	1:A:534:ALA:N	2.34	0.41
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLN:O	1:A:521:ILE:C	2.59	0.41
2:B:24:TRP:CZ3	2:B:61:PHE:CD1	3.09	0.41
2:B:242:GLN:HE21	2:B:242:GLN:CA	2.30	0.41
2:B:395:LYS:O	2:B:399:GLU:CG	2.69	0.41
1:A:178:ILE:CD1	1:A:179:VAL:N	2.74	0.41
2:B:388:LYS:HD3	2:B:388:LYS:C	2.41	0.41
1:A:402:TRP:CD1	1:A:402:TRP:C	2.90	0.41
1:A:402:TRP:HD1	2:B:331:LYS:NZ	2.17	0.41
1:A:53:GLU:O	1:A:55:PRO:HD3	2.20	0.41
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.82	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD3	1.87	0.41
1:A:319:TYR:CZ	1:A:321:PRO:HA	2.56	0.41
2:B:257:ILE:CG2	2:B:283:LEU:HD11	2.51	0.41
2:B:13:LYS:HE3	2:B:85:GLN:CB	2.38	0.41
1:A:77:PHE:O	1:A:78:ARG:C	2.59	0.40
1:A:94:ILE:CG2	1:A:95:PRO:HD2	2.47	0.40
1:A:178:ILE:HD11	1:A:180:ILE:HD13	2.03	0.40
2:B:246:LEU:HB2	2:B:307:ARG:NH1	2.36	0.40
2:B:282:LEU:HG	2:B:282:LEU:H	1.66	0.40
1:A:91:GLN:NE2	1:A:183:TYR:CD1	2.89	0.40
1:A:437:ALA:HB1	1:A:492:GLU:O	2.21	0.40
1:A:220:LYS:O	1:A:220:LYS:HG2	2.21	0.40
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.52	0.40
2:B:41:MET:HE2	2:B:47:ILE:HG23	2.04	0.40
2:B:88:TRP:CE2	2:B:154:LYS:HD2	2.56	0.40
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.22	0.40
1:A:8:VAL:O	1:A:121:ASP:HB2	2.22	0.40
1:A:17:ASP:O	1:A:83:ARG:NE	2.55	0.40
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.02	0.40
1:A:64:LYS:O	1:A:65:LYS:C	2.60	0.40
1:A:328:GLU:HG2	1:A:390:LYS:HB2	2.03	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	550/560 (98%)	501 (91%)	43 (8%)	6 (1%)	14	41
2	B	398/440 (90%)	367 (92%)	25 (6%)	6 (2%)	10	33
All	All	948/1000 (95%)	868 (92%)	68 (7%)	12 (1%)	12	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	90	VAL
2	B	65	LYS
1	A	114	ALA
1	A	543	GLY
2	B	12	LEU
2	B	238	LYS
2	B	363	ASN
1	A	443	ASP
2	B	37	ILE
2	B	346	PHE
1	A	510	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	494/500 (99%)	442 (90%)	52 (10%)	7	20
2	B	366/400 (92%)	329 (90%)	37 (10%)	7	22
All	All	860/900 (96%)	771 (90%)	89 (10%)	7	21

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

Mol	Chain	Res	Type
1	A	10	VAL

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Mol	Chain	Res	Type
1	A	11	LYS
1	A	16	MET
1	A	29	GLU
1	A	40	GLU
1	A	43	LYS
1	A	44	GLU
1	A	49	LYS
1	A	70	LYS
1	A	73	LYS
1	A	92	LEU
1	A	113	ASP
1	A	120	LEU
1	A	122	GLU
1	A	137	ASN
1	A	161	GLN
1	A	166	LYS
1	A	173	LYS
1	A	177	ASP
1	A	178	ILE
1	A	182	GLN
1	A	192	ASP
1	A	199	ARG
1	A	204	GLU
1	A	205	LEU
1	A	207	GLN
1	A	209	LEU
1	A	264	LEU
1	A	275	LYS
1	A	281	LYS
1	A	283	LEU
1	A	289	LEU
1	A	298	GLU
1	A	301	LEU
1	A	303	LEU
1	A	325	LEU
1	A	357	MET
1	A	361	HIS
1	A	374	LYS
1	A	379	SER
1	A	402	TRP
1	A	404	GLU
1	A	447	ASN

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Mol	Chain	Res	Type
1	A	476	LYS
1	A	479	LEU
1	A	503	LEU
1	A	507	GLN
1	A	517	LEU
1	A	523	GLU
1	A	527	LYS
1	A	533	LEU
1	A	539	HIS
2	B	11	LYS
2	B	16	MET
2	B	24	TRP
2	B	29	GLU
2	B	30	LYS
2	B	40	GLU
2	B	61	PHE
2	B	65	LYS
2	B	91	GLN
2	B	92	LEU
2	B	109	LEU
2	B	161	GLN
2	B	169	GLU
2	B	175	ASN
2	B	194	GLU
2	B	205	LEU
2	B	206	ARG
2	B	209	LEU
2	B	234	LEU
2	B	242	GLN
2	B	250	ASP
2	B	259	LYS
2	B	260	LEU
2	B	265	ASN
2	B	275	LYS
2	B	279	LEU
2	B	282	LEU
2	B	292	VAL
2	B	295	LEU
2	B	298	GLU
2	B	305	GLU
2	B	344	GLU
2	B	364	ASP

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Mol	Chain	Res	Type
2	B	368	LEU
2	B	388	LYS
2	B	395	LYS
2	B	414	TRP

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	145	GLN
1	A	221	HIS
1	A	258	GLN
1	A	332	GLN
1	A	336	GLN
1	A	367	GLN
1	A	373	GLN
1	A	447	ASN
1	A	475	GLN
1	A	500	GLN
1	A	512	GLN
1	A	545	ASN
2	B	91	GLN
2	B	96	HIS
2	B	197	GLN
2	B	208	HIS
2	B	242	GLN
2	B	255	ASN
2	B	334	GLN
2	B	348	ASN
2	B	394	GLN
2	B	407	GLN
2	B	418	ASN
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)

6 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	SO4	A	565	-	4,4,4	0.30	0	6,6,6	0.10	0
4	SO4	A	564	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	A	563	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	A	562	-	4,4,4	0.29	0	6,6,6	0.26	0
3	T27	A	561	-	30,30,30	2.96	15 (50%)	39,40,40	2.25	6 (15%)
4	SO4	B	441	-	4,4,4	0.32	0	6,6,6	0.25	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
3	T27	A	561	-	-	0/13/14/14	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	T27	C12-N2	6.98	1.44	1.34
3	A	561	T27	C6-C1	5.54	1.48	1.40
3	A	561	T27	C6-C5	5.13	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	T27	C11-N3	4.37	1.43	1.34
3	A	561	T27	C9-N2	4.33	1.43	1.34
3	A	561	T27	C18-C17	3.97	1.46	1.38
3	A	561	T27	C15-C16	3.92	1.45	1.39
3	A	561	T27	C2-C3	3.55	1.45	1.39
3	A	561	T27	C4-C5	3.34	1.44	1.39
3	A	561	T27	C17-C16	3.30	1.44	1.39
3	A	561	T27	C18-C13	3.24	1.46	1.39
3	A	561	T27	C12-N4	3.04	1.42	1.36
3	A	561	T27	C12-N3	2.41	1.42	1.34
3	A	561	T27	C4-C3	2.40	1.43	1.39
3	A	561	T27	C10-C9	2.00	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	561	T27	N2-C12-N3	-9.96	117.11	126.55
3	A	561	T27	C9-N2-C12	6.31	121.05	115.45
3	A	561	T27	C6-N1-C11	-3.13	118.53	124.18
3	A	561	T27	C12-N3-C11	3.01	122.27	116.28
3	A	561	T27	C10-C9-N2	-2.41	120.97	123.96
3	A	561	T27	C9-C10-C11	2.16	118.17	116.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

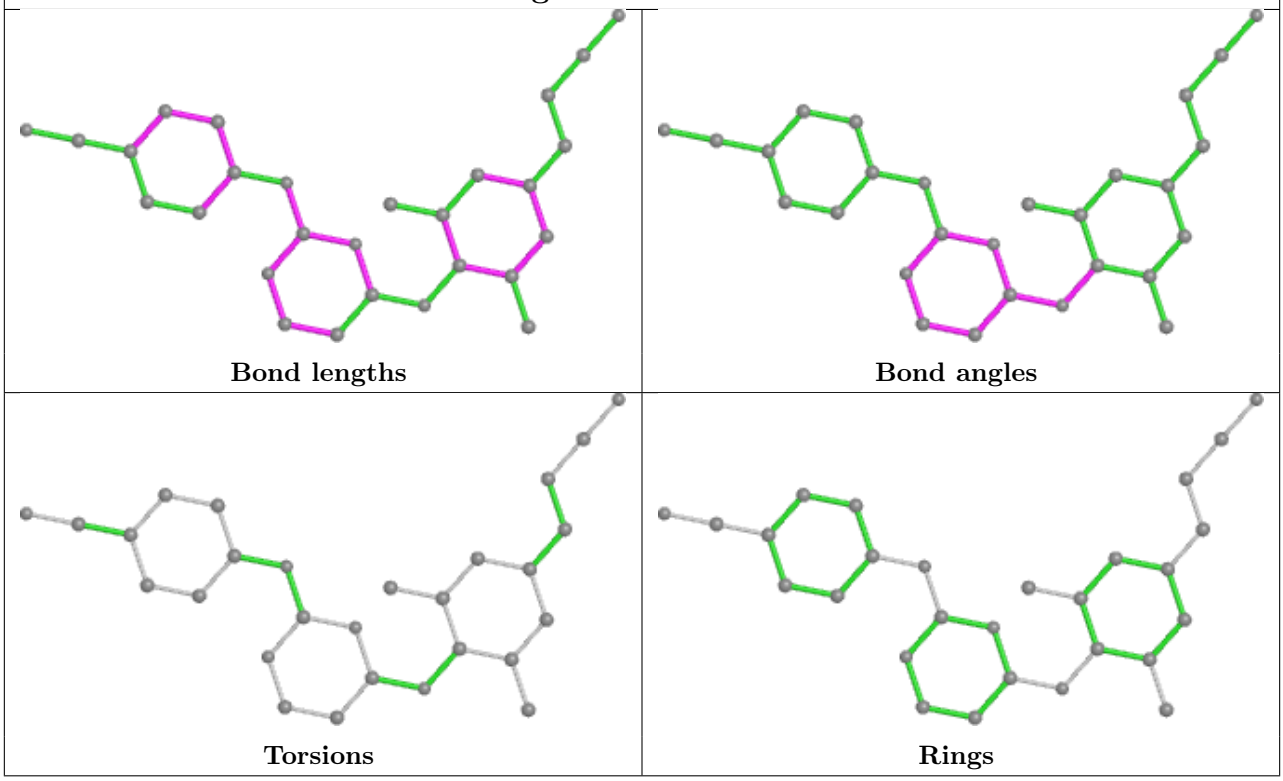
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	T27	5	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 561



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	552/560 (98%)	0.12	11 (1%)	65	56	38, 63, 100, 130	0
2	B	404/440 (91%)	0.02	9 (2%)	62	52	34, 59, 102, 118	0
All	All	956/1000 (95%)	0.08	20 (2%)	63	54	34, 62, 101, 130	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	GLN	5.4
1	A	194	GLU	3.2
2	B	88	TRP	3.1
2	B	86	ASP	2.9
2	B	252	TRP	2.9
1	A	425	LEU	2.9
1	A	193	LEU	2.8
1	A	426	TRP	2.7
2	B	361	HIS	2.7
1	A	216	THR	2.6
1	A	220	LYS	2.6
1	A	195	ILE	2.6
2	B	87	PHE	2.4
2	B	266	TRP	2.4
1	A	217	PRO	2.3
1	A	219	LYS	2.3
2	B	92	LEU	2.3
2	B	67	ASP	2.3
1	A	551	LEU	2.2
2	B	362	THR	2.1

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)

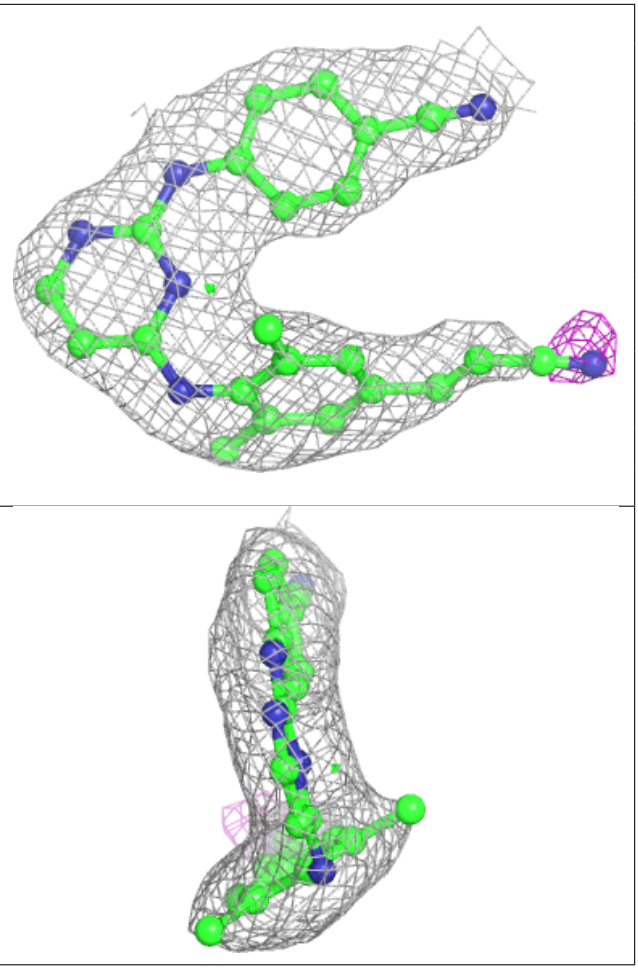
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	564	5/5	0.76	0.25	131,131,131,132	0
4	SO4	A	563	5/5	0.91	0.12	91,92,94,95	0
4	SO4	A	565	5/5	0.92	0.14	113,113,113,114	0
3	T27	A	561	28/28	0.95	0.26	36,44,66,76	0
4	SO4	B	441	5/5	0.95	0.17	110,110,110,111	0
4	SO4	A	562	5/5	0.96	0.15	64,66,68,69	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 561:

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.