



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:18 AM EDT

PDB ID : 1TV6 / pdb_00001tv6
Title : HIV-1 Reverse Transcriptase Complexed with CP-94,707
Authors : Pata, J.D.; Stirtan, W.G.; Goldstein, S.W.; Steitz, T.A.
Deposited on : 2004-06-28
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

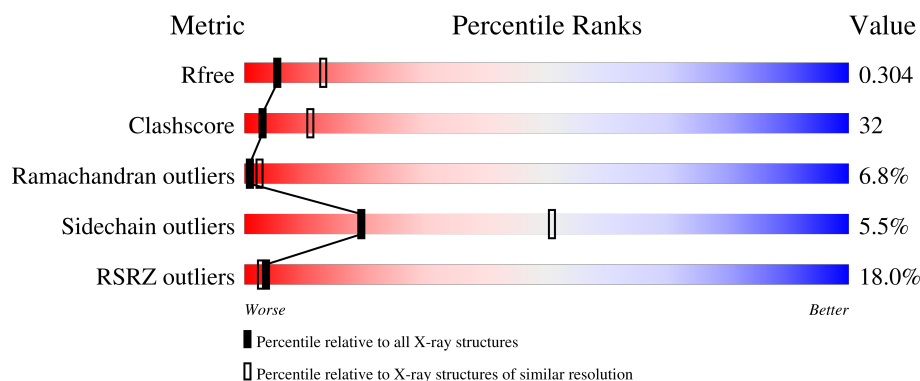
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7786 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.

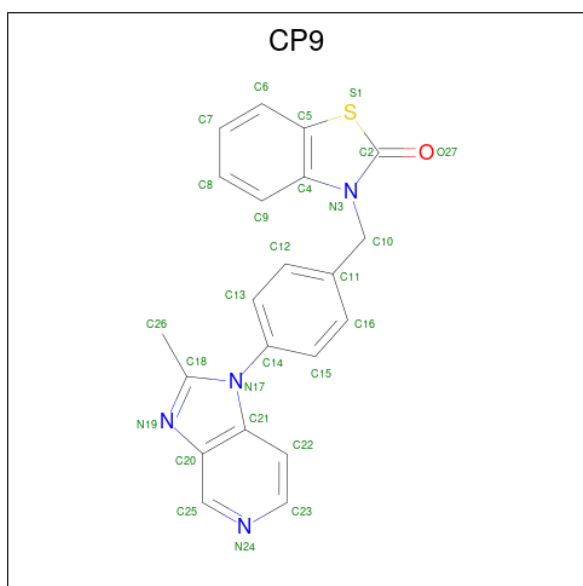
- Molecule 1 is a protein called reverse transcriptase p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4367	2832	722	805	8			

- Molecule 2 is a protein called reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	411	Total	C	N	O	S	0	0	0
			3392	2205	562	618	7			

- Molecule 3 is 3-[4-(2-METHYL-IMIDAZO[4,5-C]PYRIDIN-1-YL)BENZYL]-3H-BENZOTHIADIAZOL-2-ONE (CCD ID: CP9) (formula: C₂₁H₁₆N₄OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	21	4	1	1		

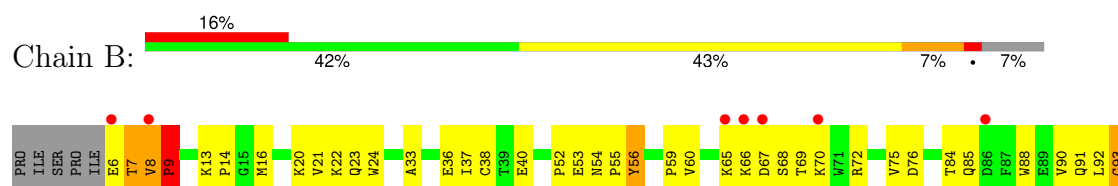
3 Residue-property plots

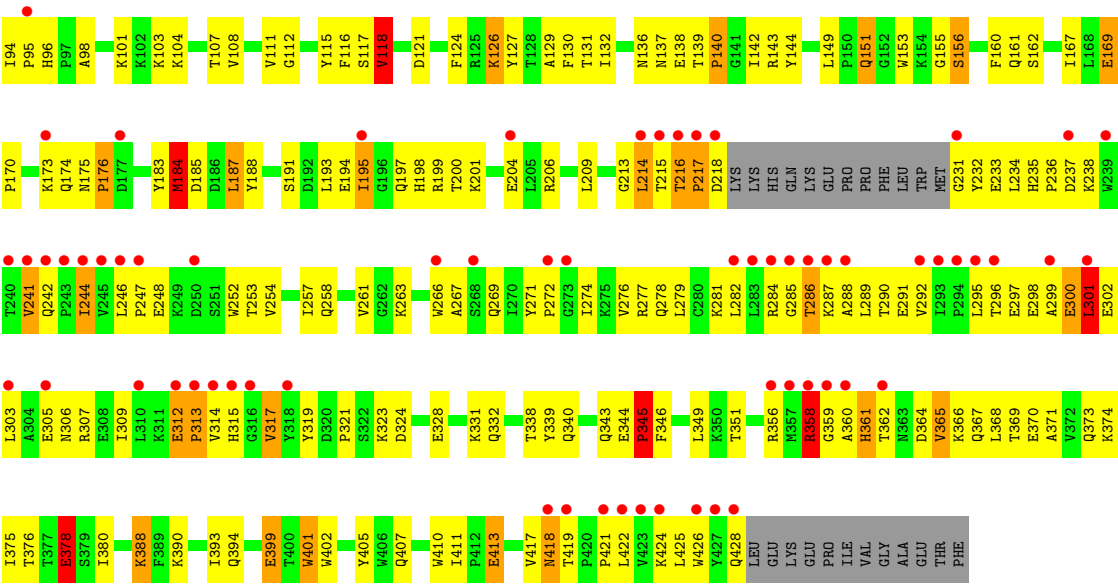
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: reverse transcriptase p66 subunit



• Molecule 2: reverse transcriptase p51 subunit





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.91Å 69.04Å 104.33Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.00-2.80) 94.4 (30.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.312 0.256 , 0.304	Depositor DCC
R_{free} test set	1995 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7786	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: CP9

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	0.52	0/4483	1.08	35/6094 (0.6%)
2	B	0.62	0/3488	1.11	31/4740 (0.7%)
All	All	0.56	0/7971	1.09	66/10834 (0.6%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	LYS	N-CA-C	12.18	128.30	110.28
1	A	53	GLU	N-CA-C	9.70	124.16	110.68
1	A	227	PHE	N-CA-C	9.62	123.23	110.53
2	B	358	ARG	N-CA-C	7.92	127.68	110.80
1	A	13	LYS	CA-C-N	7.77	129.56	119.84
1	A	13	LYS	C-N-CA	7.77	129.56	119.84
2	B	233	GLU	N-CA-C	7.44	120.20	108.67
1	A	349	LEU	N-CA-C	-6.96	103.14	111.69
2	B	418	ASN	N-CA-C	6.83	121.51	107.37
1	A	348	ASN	N-CA-C	6.73	119.99	110.50
2	B	96	HIS	CA-C-N	6.71	128.23	119.84
2	B	96	HIS	C-N-CA	6.71	128.23	119.84
1	A	499	SER	N-CA-C	6.68	119.62	108.20
2	B	312	GLU	CA-C-N	6.66	128.16	119.84
2	B	312	GLU	C-N-CA	6.66	128.16	119.84
1	A	225	PRO	N-CA-C	6.58	118.73	110.70
1	A	246	LEU	CA-C-N	6.47	126.49	119.89
1	A	246	LEU	C-N-CA	6.47	126.49	119.89
1	A	235	HIS	CA-C-N	6.29	125.99	119.82
1	A	235	HIS	C-N-CA	6.29	125.99	119.82
1	A	382	ILE	N-CA-C	6.22	116.85	110.82
1	A	149	LEU	CA-C-N	6.17	127.82	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	LEU	C-N-CA	6.17	127.82	120.23
1	A	67	ASP	N-CA-C	6.08	119.80	112.38
1	A	476	LYS	N-CA-C	-6.05	104.77	111.36
1	A	423	VAL	N-CA-C	5.98	117.19	108.58
1	A	281	LYS	N-CA-C	-5.86	105.39	112.54
2	B	269	GLN	N-CA-C	-5.84	106.15	113.28
2	B	411	ILE	CA-C-N	-5.72	112.68	119.84
2	B	411	ILE	C-N-CA	-5.72	112.68	119.84
2	B	301	LEU	N-CA-C	-5.71	106.35	113.15
1	A	29	GLU	N-CA-C	-5.66	105.25	111.82
1	A	233	GLU	N-CA-C	-5.65	100.60	109.25
1	A	197	GLN	N-CA-C	-5.56	105.30	111.36
1	A	391	LEU	N-CA-C	5.55	119.20	109.48
2	B	359	GLY	N-CA-C	5.53	119.20	110.96
2	B	184	MET	CB-CA-C	-5.53	109.71	117.23
1	A	50	ILE	N-CA-C	5.52	117.86	108.86
2	B	140	PRO	N-CA-C	5.47	121.13	113.53
1	A	475	GLN	N-CA-C	-5.46	107.16	113.88
1	A	175	ASN	CA-C-N	5.46	125.81	119.47
1	A	175	ASN	C-N-CA	5.46	125.81	119.47
2	B	378	GLU	N-CA-C	-5.43	105.36	111.28
2	B	204	GLU	N-CA-C	-5.42	105.28	111.14
1	A	388	LYS	N-CA-C	-5.42	100.46	109.46
2	B	118	VAL	CA-C-N	5.40	125.38	120.03
2	B	118	VAL	C-N-CA	5.40	125.38	120.03
2	B	344	GLU	CA-C-N	5.35	126.53	119.84
2	B	344	GLU	C-N-CA	5.35	126.53	119.84
2	B	238	LYS	N-CA-C	-5.33	106.78	113.72
2	B	235	HIS	CA-C-N	5.25	125.31	119.32
2	B	235	HIS	C-N-CA	5.25	125.31	119.32
1	A	481	ALA	N-CA-C	-5.24	105.22	111.03
1	A	132	ILE	CA-C-N	5.24	126.38	119.84
1	A	132	ILE	C-N-CA	5.24	126.38	119.84
1	A	68	SER	N-CA-C	5.21	119.63	113.12
2	B	401	TRP	N-CA-C	5.18	120.45	113.72
2	B	365	VAL	N-CA-C	5.13	115.75	110.36
1	A	319	TYR	N-CA-C	5.13	117.97	109.46
2	B	8	VAL	CA-C-N	5.12	126.24	119.84
2	B	8	VAL	C-N-CA	5.12	126.24	119.84
1	A	147	ASN	N-CA-C	-5.10	105.95	113.61
2	B	56	TYR	N-CA-C	5.10	117.44	110.55
2	B	169	GLU	CA-C-N	5.09	124.81	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	GLU	C-N-CA	5.09	124.81	119.82
2	B	69	THR	N-CA-C	-5.04	106.44	112.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4367	0	4419	314	0
2	B	3392	0	3418	195	0
3	A	27	0	16	8	0
All	All	7786	0	7853	499	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 32.

All (499) 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:362:THR:HG22	1:A:363:ASN:H	1.12	1.15
2:B:65:LYS:HE3	2:B:72:ARG:HD2	1.24	1.08
1:A:92:LEU:HD23	1:A:93:GLY:H	1.16	1.07
2:B:195:ILE:HG22	2:B:199:ARG:HE	1.19	1.04
1:A:424:LYS:HD2	1:A:426:TRP:HE1	1.22	1.01
1:A:236:PRO:HA	3:A:561:CP9:N24	1.77	0.99
1:A:130:PHE:CE2	1:A:144:TYR:HB2	2.01	0.96
2:B:244:ILE:HD12	2:B:244:ILE:H	1.28	0.95
2:B:241:VAL:HG12	2:B:242:GLN:H	1.28	0.95
1:A:424:LYS:HD2	1:A:426:TRP:NE1	1.82	0.95
1:A:362:THR:HG22	1:A:363:ASN:N	1.87	0.90
1:A:228:LEU:H	1:A:228:LEU:HD23	1.33	0.90
2:B:195:ILE:CG2	2:B:199:ARG:HE	1.86	0.88
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.58	0.86
1:A:28:GLU:O	1:A:32:LYS:HG2	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HG22	1:A:29:GLU:H	1.38	0.85
1:A:130:PHE:H	1:A:130:PHE:HD2	1.24	0.85
1:A:362:THR:CG2	1:A:363:ASN:H	1.89	0.84
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.18	0.84
1:A:92:LEU:HD23	1:A:93:GLY:N	1.93	0.82
2:B:139:THR:HB	2:B:140:PRO:HD2	1.63	0.81
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.62	0.81
1:A:334:GLN:HE22	1:A:512:LYS:HG3	1.47	0.80
2:B:149:LEU:HB3	2:B:156:SER:OG	1.82	0.79
1:A:193:LEU:HD12	1:A:198:HIS:HA	1.64	0.79
1:A:23:GLN:HE22	1:A:60:VAL:HG23	1.48	0.79
1:A:445:ALA:HA	1:A:474:ASN:ND2	1.98	0.79
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.63	0.78
2:B:213:GLY:O	2:B:215:THR:N	2.16	0.78
1:A:459:THR:HG22	1:A:463:ARG:O	1.84	0.78
2:B:356:ARG:HE	2:B:358:ARG:HG2	1.49	0.78
1:A:424:LYS:HE3	1:A:511:ASP:HB2	1.65	0.77
2:B:126:LYS:HE2	2:B:127:TYR:CZ	2.20	0.76
2:B:232:TYR:HE2	2:B:234:LEU:HD21	1.49	0.76
2:B:324:ASP:O	2:B:343:GLN:HG2	1.87	0.75
1:A:358:ARG:H	1:A:358:ARG:HD3	1.51	0.75
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.67	0.74
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.67	0.74
2:B:281:LYS:HA	2:B:284:ARG:HD3	1.69	0.74
2:B:218:ASP:C	2:B:231:GLY:N	2.46	0.74
2:B:142:ILE:H	2:B:142:ILE:HD12	1.53	0.74
2:B:328:GLU:HG2	2:B:390:LYS:HG3	1.70	0.73
3:A:561:CP9:H15	3:A:561:CP9:H263	1.68	0.73
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.70	0.72
1:A:519:ASN:O	1:A:523:GLU:HG2	1.88	0.72
1:A:317:VAL:HG12	1:A:348:ASN:O	1.89	0.72
2:B:252:TRP:CD1	2:B:295:LEU:HD21	2.24	0.72
2:B:241:VAL:HG12	2:B:242:GLN:N	2.05	0.72
2:B:305:GLU:O	2:B:309:ILE:HG13	1.89	0.72
1:A:459:THR:HG21	1:A:463:ARG:HB3	1.72	0.71
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.26	0.70
2:B:279:LEU:HD23	2:B:282:LEU:HD12	1.73	0.70
1:A:30:LYS:HG2	1:A:71:TRP:CZ3	2.27	0.70
1:A:253:THR:HB	1:A:290:THR:HA	1.74	0.70
3:A:561:CP9:H22	3:A:561:CP9:H13	1.73	0.69
2:B:195:ILE:HG22	2:B:199:ARG:NE	2.00	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.73	0.68
1:A:400:THR:O	1:A:404:GLU:HG2	1.94	0.68
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.08	0.68
1:A:479:LEU:HB3	1:A:517:LEU:HD21	1.76	0.68
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.76	0.68
1:A:301:LEU:O	1:A:305:GLU:HG2	1.94	0.67
2:B:303:LEU:O	2:B:307:ARG:HG3	1.95	0.67
1:A:29:GLU:O	1:A:32:LYS:HB2	1.94	0.66
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.29	0.66
1:A:459:THR:CG2	1:A:463:ARG:H	2.09	0.66
1:A:382:ILE:HA	2:B:136:ASN:HD22	1.59	0.66
1:A:134:SER:HB3	1:A:139:THR:O	1.95	0.66
2:B:197:GLN:O	2:B:200:THR:HB	1.96	0.66
2:B:246:LEU:HD12	2:B:307:ARG:HG2	1.78	0.65
1:A:132:ILE:HB	1:A:142:ILE:CG2	2.27	0.65
1:A:445:ALA:HA	1:A:474:ASN:HD21	1.60	0.65
1:A:303:LEU:O	1:A:307:ARG:HG3	1.95	0.65
1:A:424:LYS:HE3	1:A:511:ASP:CB	2.27	0.65
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.78	0.65
1:A:171:PHE:HB2	1:A:208:HIS:CE1	2.31	0.65
1:A:254:VAL:HG13	1:A:283:LEU:HD22	1.78	0.65
1:A:57:ASN:HA	1:A:129:ALA:O	1.96	0.64
1:A:515:SER:O	1:A:517:LEU:N	2.30	0.64
2:B:369:THR:HG22	2:B:373:GLN:NE2	2.12	0.64
1:A:269:GLN:HA	1:A:351:THR:O	1.96	0.64
2:B:248:GLU:HB2	2:B:307:ARG:NH1	2.12	0.64
1:A:364:ASP:OD2	1:A:424:LYS:NZ	2.29	0.64
2:B:214:LEU:O	2:B:216:THR:HG22	1.97	0.64
2:B:244:ILE:H	2:B:244:ILE:CD1	2.06	0.64
1:A:132:ILE:HB	1:A:142:ILE:HG21	1.80	0.63
1:A:226:PRO:HA	1:A:234:LEU:O	1.99	0.63
2:B:242:GLN:O	2:B:242:GLN:HG3	1.96	0.63
1:A:424:LYS:HB2	1:A:426:TRP:NE1	2.14	0.63
1:A:424:LYS:HZ2	1:A:511:ASP:HB3	1.62	0.62
1:A:460:ASN:HA	2:B:286:THR:HG22	1.80	0.62
1:A:62:ALA:O	1:A:63:ILE:HD13	2.00	0.62
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.99	0.62
1:A:31:ILE:O	1:A:35:VAL:HG23	1.98	0.62
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.82	0.62
1:A:132:ILE:O	1:A:142:ILE:HB	1.99	0.62
1:A:392:PRO:O	1:A:423:VAL:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:HB3	1:A:240:THR:HG23	1.81	0.62
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.34	0.62
1:A:320:ASP:C	1:A:322:SER:H	2.09	0.61
1:A:1:PRO:HG2	1:A:213:GLY:O	2.01	0.61
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.35	0.61
2:B:142:ILE:HD12	2:B:142:ILE:N	2.15	0.61
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.35	0.61
1:A:88:TRP:CZ3	2:B:22:LYS:NZ	2.69	0.60
1:A:254:VAL:O	1:A:258:GLN:HG3	2.00	0.60
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.35	0.60
1:A:171:PHE:HB2	1:A:208:HIS:ND1	2.17	0.60
2:B:241:VAL:CG1	2:B:242:GLN:H	2.10	0.60
2:B:13:LYS:O	2:B:16:MET:HB2	2.00	0.60
2:B:174:GLN:C	2:B:176:PRO:HD3	2.26	0.60
1:A:235:HIS:CD2	1:A:238:LYS:HE3	2.35	0.60
1:A:30:LYS:C	1:A:32:LYS:H	2.08	0.60
1:A:424:LYS:CD	1:A:426:TRP:HE1	2.06	0.60
1:A:442:VAL:O	1:A:443:ASP:HB3	2.00	0.60
2:B:33:ALA:O	2:B:36:GLU:HG2	2.02	0.60
1:A:459:THR:CG2	1:A:463:ARG:HB3	2.30	0.60
1:A:130:PHE:CD2	1:A:130:PHE:N	2.69	0.59
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.84	0.59
1:A:130:PHE:HD2	1:A:130:PHE:N	1.97	0.59
1:A:512:LYS:C	1:A:514:GLU:H	2.09	0.59
1:A:112:GLY:C	1:A:114:ALA:H	2.09	0.59
2:B:115:TYR:HE2	2:B:185:ASP:OD1	1.85	0.59
2:B:118:VAL:HG22	2:B:149:LEU:HG	1.85	0.59
2:B:232:TYR:CE2	2:B:234:LEU:HD21	2.36	0.59
2:B:314:VAL:HG22	2:B:315:HIS:N	2.18	0.59
1:A:270:ILE:HG23	1:A:271:TYR:CD2	2.38	0.59
2:B:282:LEU:HD21	2:B:296:THR:CG2	2.33	0.58
1:A:25:PRO:O	1:A:26:LEU:HD23	2.02	0.58
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.38	0.58
1:A:88:TRP:HZ3	2:B:22:LYS:NZ	2.02	0.58
1:A:326:ILE:HD13	1:A:388:LYS:HB2	1.84	0.58
1:A:424:LYS:HD2	1:A:426:TRP:CD1	2.37	0.58
1:A:457:TYR:CD1	1:A:457:TYR:C	2.80	0.58
2:B:8:VAL:HG12	2:B:8:VAL:O	2.02	0.58
1:A:30:LYS:C	1:A:32:LYS:N	2.62	0.58
1:A:73:LYS:NZ	1:A:130:PHE:HE1	2.02	0.58
2:B:360:ALA:O	2:B:361:HIS:CG	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ILE:HG23	2:B:136:ASN:ND2	2.19	0.57
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.86	0.57
1:A:427:TYR:OH	1:A:509:GLN:HA	2.04	0.57
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.39	0.57
2:B:242:GLN:HB3	2:B:351:THR:OG1	2.04	0.57
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.69	0.57
1:A:27:THR:HG22	1:A:29:GLU:N	2.13	0.57
2:B:115:TYR:C	2:B:117:SER:H	2.13	0.57
1:A:89:GLU:O	1:A:91:GLN:N	2.38	0.57
1:A:68:SER:O	1:A:69:THR:HG23	2.04	0.57
1:A:252:TRP:CD1	1:A:295:LEU:HD21	2.40	0.57
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.04	0.56
1:A:41:MET:HE2	1:A:47:ILE:HD13	1.85	0.56
1:A:334:GLN:HE22	1:A:512:LYS:CG	2.18	0.56
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.35	0.56
2:B:214:LEU:O	2:B:216:THR:N	2.38	0.56
1:A:2:ILE:HD11	1:A:119:PRO:HB3	1.87	0.56
1:A:358:ARG:HD3	1:A:358:ARG:N	2.20	0.56
1:A:535:TRP:CZ3	2:B:422:LEU:HD11	2.40	0.56
2:B:369:THR:HG22	2:B:373:GLN:HE22	1.71	0.56
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.41	0.56
2:B:244:ILE:HD12	2:B:244:ILE:N	2.11	0.56
2:B:248:GLU:HB2	2:B:307:ARG:CZ	2.36	0.56
2:B:366:LYS:HA	2:B:405:TYR:CD2	2.41	0.56
1:A:88:TRP:O	1:A:89:GLU:C	2.49	0.55
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.35	0.55
2:B:76:ASP:OD1	2:B:76:ASP:C	2.48	0.55
1:A:459:THR:CG2	1:A:463:ARG:N	2.69	0.55
1:A:188:TYR:HB2	3:A:561:CP9:S1	2.46	0.55
1:A:324:ASP:O	1:A:343:GLN:HG2	2.07	0.55
2:B:425:LEU:HD12	2:B:428:GLN:OE1	2.05	0.55
2:B:194:GLU:O	2:B:195:ILE:C	2.48	0.55
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.37	0.55
2:B:213:GLY:C	2:B:215:THR:H	2.15	0.55
1:A:416:PHE:CD1	1:A:417:VAL:N	2.75	0.55
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.06	0.55
2:B:276:VAL:C	2:B:278:GLN:H	2.14	0.55
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.89	0.54
1:A:72:ARG:HD3	1:A:73:LYS:O	2.08	0.54
2:B:92:LEU:O	2:B:93:GLY:O	2.25	0.54
1:A:191:SER:OG	1:A:198:HIS:ND1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HD21	1:A:303:LEU:CD1	2.37	0.54
1:A:281:LYS:O	1:A:284:ARG:HG3	2.06	0.54
1:A:324:ASP:OD1	1:A:388:LYS:HE3	2.08	0.54
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.90	0.54
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.43	0.54
1:A:164:MET:HE2	1:A:187:LEU:HD21	1.89	0.54
1:A:472:THR:OG1	1:A:476:LYS:HB3	2.08	0.54
2:B:209:LEU:HD12	2:B:217:PRO:HG2	1.90	0.54
2:B:254:VAL:HG21	2:B:288:ALA:O	2.08	0.54
1:A:489:SER:HB3	1:A:493:VAL:HG22	1.89	0.54
1:A:28:GLU:O	1:A:28:GLU:HG2	2.07	0.54
1:A:228:LEU:H	1:A:228:LEU:CD2	2.11	0.54
1:A:130:PHE:HE2	1:A:144:TYR:HB2	1.67	0.53
1:A:194:GLU:H	1:A:197:GLN:HB3	1.73	0.53
1:A:23:GLN:NE2	1:A:60:VAL:HG23	2.19	0.53
1:A:368:LEU:O	1:A:372:VAL:HG23	2.08	0.53
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.24	0.53
1:A:296:THR:HG22	1:A:298:GLU:H	1.73	0.53
1:A:356:ARG:NE	1:A:359:GLY:HA3	2.23	0.53
1:A:359:GLY:O	1:A:361:HIS:N	2.42	0.53
1:A:510:PRO:HG2	1:A:522:ILE:HD11	1.89	0.53
1:A:30:LYS:HG2	1:A:71:TRP:CH2	2.44	0.53
1:A:188:TYR:CD2	1:A:188:TYR:C	2.87	0.53
1:A:395:LYS:HG3	1:A:414:TRP:CH2	2.44	0.53
1:A:447:ASN:OD1	1:A:449:GLU:HB2	2.08	0.53
1:A:511:ASP:OD2	1:A:512:LYS:HG2	2.09	0.53
1:A:100:LEU:HD13	3:A:561:CP9:H16	1.90	0.53
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.91	0.52
1:A:277:ARG:CB	1:A:336:GLN:NE2	2.73	0.52
1:A:224:GLU:O	1:A:226:PRO:N	2.42	0.52
1:A:503:LEU:O	1:A:507:GLN:HG3	2.09	0.52
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.92	0.52
2:B:169:GLU:OE1	2:B:173:LYS:HE2	2.08	0.52
1:A:62:ALA:C	1:A:63:ILE:HD13	2.34	0.52
1:A:493:VAL:HG12	1:A:494:ASN:N	2.24	0.52
2:B:7:THR:HG23	2:B:121:ASP:HB2	1.91	0.52
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.75	0.52
2:B:191:SER:OG	2:B:198:HIS:ND1	2.35	0.52
1:A:356:ARG:CZ	1:A:359:GLY:HA3	2.40	0.52
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.91	0.51
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:GLU:O	1:A:532:TYR:HD1	1.94	0.51
1:A:452:LEU:HD23	1:A:470:THR:HA	1.92	0.51
2:B:24:TRP:CZ3	2:B:399:GLU:HG2	2.46	0.51
1:A:108:VAL:HA	1:A:187:LEU:O	2.10	0.51
1:A:225:PRO:O	1:A:227:PHE:N	2.40	0.51
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.92	0.51
2:B:94:ILE:HD11	2:B:161:GLN:HG2	1.92	0.51
1:A:320:ASP:O	1:A:322:SER:N	2.44	0.51
1:A:60:VAL:C	1:A:61:PHE:HD1	2.18	0.51
1:A:305:GLU:O	1:A:309:ILE:HG13	2.10	0.51
2:B:331:LYS:O	2:B:424:LYS:HD2	2.11	0.51
1:A:297:GLU:O	1:A:300:GLU:HG2	2.11	0.51
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.92	0.51
1:A:424:LYS:HB2	1:A:426:TRP:CD1	2.46	0.51
2:B:276:VAL:C	2:B:278:GLN:N	2.67	0.51
1:A:90:VAL:O	1:A:91:GLN:C	2.53	0.51
1:A:180:ILE:O	1:A:181:TYR:HD2	1.94	0.50
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.50	0.50
2:B:271:TYR:HB2	2:B:274:ILE:HD12	1.94	0.50
1:A:111:VAL:HG23	1:A:111:VAL:O	2.10	0.50
1:A:112:GLY:O	1:A:114:ALA:N	2.40	0.50
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.92	0.50
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.92	0.50
1:A:238:LYS:HD2	1:A:315:HIS:HB3	1.94	0.50
2:B:52:PRO:C	2:B:54:ASN:H	2.20	0.50
1:A:489:SER:HB3	1:A:493:VAL:CG2	2.42	0.50
2:B:365:VAL:HG12	2:B:405:TYR:HE2	1.77	0.50
1:A:511:ASP:OD2	1:A:512:LYS:N	2.44	0.50
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.45	0.50
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.94	0.50
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.40	0.50
1:A:276:VAL:HG12	1:A:276:VAL:O	2.12	0.49
1:A:317:VAL:HG22	1:A:318:TYR:N	2.27	0.49
2:B:115:TYR:C	2:B:117:SER:N	2.69	0.49
2:B:366:LYS:O	2:B:370:GLU:HG3	2.13	0.49
1:A:377:THR:O	1:A:381:VAL:HG23	2.13	0.49
2:B:213:GLY:C	2:B:215:THR:N	2.70	0.49
1:A:136:ASN:O	1:A:138:GLU:N	2.45	0.49
1:A:424:LYS:CB	1:A:426:TRP:NE1	2.75	0.49
1:A:457:TYR:C	1:A:457:TYR:HD1	2.19	0.49
2:B:257:ILE:O	2:B:261:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.95	0.49
1:A:512:LYS:HZ1	1:A:523:GLU:CD	2.20	0.49
2:B:300:GLU:C	2:B:302:GLU:H	2.20	0.49
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.48	0.49
1:A:140:PRO:O	1:A:142:ILE:N	2.46	0.49
2:B:160:PHE:O	2:B:161:GLN:C	2.56	0.49
2:B:297:GLU:C	2:B:299:ALA:H	2.20	0.49
1:A:217:PRO:O	1:A:218:ASP:O	2.31	0.49
1:A:513:SER:O	1:A:514:GLU:C	2.55	0.48
2:B:66:LYS:HE3	2:B:67:ASP:OD1	2.12	0.48
1:A:181:TYR:CE1	2:B:138:GLU:HB3	2.49	0.48
2:B:266:TRP:CD1	2:B:422:LEU:HD12	2.48	0.48
1:A:94:ILE:HG13	1:A:94:ILE:O	2.11	0.48
1:A:326:ILE:CD1	1:A:388:LYS:HB2	2.43	0.48
2:B:254:VAL:O	2:B:258:GLN:HG3	2.12	0.48
2:B:425:LEU:O	2:B:428:GLN:HG2	2.13	0.48
1:A:320:ASP:C	1:A:322:SER:N	2.72	0.48
2:B:66:LYS:HA	2:B:407:GLN:OE1	2.13	0.48
2:B:136:ASN:O	2:B:137:ASN:HB2	2.12	0.48
2:B:195:ILE:O	2:B:199:ARG:HD2	2.14	0.48
2:B:13:LYS:HE3	2:B:16:MET:SD	2.54	0.48
1:A:180:ILE:O	1:A:181:TYR:CD2	2.66	0.48
1:A:538:ALA:O	1:A:539:HIS:HB2	2.13	0.48
2:B:7:THR:CG2	2:B:121:ASP:HA	2.44	0.48
2:B:242:GLN:HB3	2:B:351:THR:HG1	1.78	0.48
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.49	0.48
1:A:112:GLY:C	1:A:114:ALA:N	2.70	0.48
1:A:235:HIS:CB	1:A:236:PRO:HD2	2.38	0.48
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.96	0.48
2:B:278:GLN:HE21	2:B:301:LEU:CD2	2.27	0.47
1:A:227:PHE:HD2	1:A:228:LEU:HD23	1.79	0.47
2:B:101:LYS:O	2:B:236:PRO:HB2	2.14	0.47
1:A:236:PRO:HA	3:A:561:CP9:C25	2.43	0.47
1:A:459:THR:HG22	1:A:463:ARG:N	2.28	0.47
1:A:90:VAL:CG2	1:A:157:PRO:HB2	2.39	0.47
2:B:115:TYR:O	2:B:117:SER:N	2.48	0.47
1:A:364:ASP:CG	1:A:424:LYS:HZ3	2.21	0.47
1:A:376:THR:O	1:A:380:ILE:HG13	2.14	0.47
2:B:56:TYR:CE2	2:B:126:LYS:HD2	2.50	0.47
2:B:374:LYS:HE2	2:B:378:GLU:CD	2.40	0.47
1:A:31:ILE:HD13	1:A:133:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:THR:OG1	1:A:143:ARG:HG2	2.14	0.47
1:A:206:ARG:CZ	1:A:206:ARG:HB3	2.44	0.47
3:A:561:CP9:H13	3:A:561:CP9:C22	2.44	0.47
2:B:72:ARG:NH2	2:B:151:GLN:HE22	2.11	0.47
2:B:161:GLN:O	2:B:162:SER:C	2.58	0.47
2:B:263:LYS:HB3	2:B:426:TRP:CZ3	2.50	0.47
1:A:358:ARG:HG2	1:A:360:ALA:H	1.79	0.47
1:A:198:HIS:O	1:A:202:ILE:HG12	2.15	0.47
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.97	0.47
1:A:19:PRO:CD	1:A:80:LEU:HD13	2.45	0.47
1:A:202:ILE:O	1:A:206:ARG:HG3	2.15	0.47
2:B:276:VAL:O	2:B:278:GLN:N	2.48	0.47
1:A:240:THR:OG1	1:A:241:VAL:N	2.48	0.46
1:A:479:LEU:CB	1:A:517:LEU:HD21	2.45	0.46
1:A:31:ILE:O	1:A:31:ILE:HG22	2.14	0.46
1:A:398:TRP:CZ3	1:A:402:TRP:CD1	3.04	0.46
1:A:536:VAL:O	1:A:537:PRO:C	2.57	0.46
1:A:53:GLU:O	1:A:55:PRO:HD3	2.14	0.46
1:A:164:MET:CE	1:A:187:LEU:HD21	2.45	0.46
1:A:270:ILE:O	1:A:314:VAL:HG11	2.15	0.46
2:B:101:LYS:O	2:B:236:PRO:CB	2.64	0.46
1:A:402:TRP:CE3	1:A:402:TRP:C	2.92	0.46
2:B:94:ILE:HG12	2:B:161:GLN:OE1	2.16	0.46
2:B:339:TYR:C	2:B:340:GLN:NE2	2.74	0.46
1:A:101:LYS:HB2	1:A:101:LYS:HZ3	1.81	0.46
2:B:356:ARG:HD3	2:B:367:GLN:NE2	2.31	0.46
1:A:65:LYS:O	1:A:66:LYS:C	2.58	0.46
1:A:180:ILE:HA	1:A:188:TYR:O	2.16	0.46
2:B:184:MET:HB3	2:B:185:ASP:H	1.51	0.46
1:A:73:LYS:HZ1	1:A:130:PHE:HE1	1.63	0.46
1:A:358:ARG:HG2	1:A:359:GLY:N	2.31	0.46
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.16	0.46
1:A:297:GLU:HA	1:A:300:GLU:HG2	1.96	0.46
1:A:417:VAL:O	1:A:417:VAL:HG12	2.15	0.46
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.51	0.46
1:A:64:LYS:HD3	1:A:66:LYS:HA	1.98	0.45
3:A:561:CP9:H15	3:A:561:CP9:C26	2.40	0.45
1:A:270:ILE:HG23	1:A:271:TYR:HD2	1.79	0.45
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.44	0.45
1:A:10:VAL:HG12	1:A:11:LYS:N	2.31	0.45
1:A:115:TYR:OH	1:A:151:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LYS:HG3	2:B:413:GLU:HB3	1.98	0.45
1:A:395:LYS:HA	1:A:414:TRP:CH2	2.49	0.45
2:B:115:TYR:N	2:B:115:TYR:CD1	2.83	0.45
2:B:390:LYS:HB3	2:B:417:VAL:CG1	2.47	0.45
1:A:194:GLU:O	1:A:197:GLN:N	2.50	0.45
1:A:268:SER:C	1:A:270:ILE:H	2.24	0.45
2:B:267:ALA:HB2	2:B:426:TRP:CZ2	2.51	0.45
2:B:278:GLN:HE21	2:B:301:LEU:HD21	1.81	0.45
1:A:120:LEU:O	1:A:121:ASP:C	2.59	0.45
1:A:257:ILE:O	1:A:261:VAL:HG23	2.17	0.45
1:A:54:ASN:HD21	1:A:126:LYS:HB2	1.81	0.45
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.97	0.45
1:A:320:ASP:CG	1:A:323:LYS:NZ	2.74	0.45
1:A:30:LYS:O	1:A:32:LYS:N	2.49	0.44
1:A:68:SER:O	1:A:69:THR:CB	2.65	0.44
1:A:512:LYS:NZ	1:A:523:GLU:OE1	2.48	0.44
2:B:297:GLU:C	2:B:299:ALA:N	2.75	0.44
2:B:319:TYR:O	2:B:321:PRO:HD3	2.17	0.44
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.00	0.44
1:A:328:GLU:O	1:A:339:TYR:HA	2.17	0.44
1:A:334:GLN:NE2	1:A:512:LYS:HB2	2.33	0.44
1:A:424:LYS:NZ	1:A:511:ASP:HB3	2.30	0.44
1:A:459:THR:HG22	1:A:463:ARG:C	2.40	0.44
2:B:24:TRP:CD1	2:B:24:TRP:N	2.85	0.44
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.52	0.44
1:A:3:SER:OG	1:A:4:PRO:HD2	2.17	0.44
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.31	0.44
1:A:64:LYS:HE3	1:A:69:THR:HA	1.99	0.44
1:A:320:ASP:OD2	1:A:323:LYS:NZ	2.50	0.44
2:B:6:GLU:O	2:B:7:THR:O	2.34	0.44
2:B:312:GLU:HA	2:B:313:PRO:HD2	1.69	0.44
2:B:115:TYR:CE2	2:B:185:ASP:OD1	2.70	0.44
1:A:424:LYS:O	1:A:424:LYS:HG3	2.17	0.44
1:A:347:LYS:HA	1:A:347:LYS:HD2	1.61	0.44
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.44
1:A:193:LEU:HB3	1:A:197:GLN:OE1	2.18	0.44
2:B:104:LYS:HA	2:B:237:ASP:OD1	2.17	0.44
1:A:60:VAL:C	1:A:61:PHE:CD1	2.95	0.44
1:A:137:ASN:OD1	1:A:137:ASN:O	2.35	0.43
2:B:7:THR:HG23	2:B:121:ASP:CB	2.47	0.43
2:B:111:VAL:CG1	2:B:187:LEU:HD22	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:LYS:HA	2:B:201:LYS:HD3	1.78	0.43
1:A:126:LYS:C	1:A:128:THR:H	2.27	0.43
1:A:358:ARG:NE	1:A:359:GLY:H	2.16	0.43
1:A:374:LYS:O	1:A:374:LYS:HD3	2.18	0.43
1:A:465:LYS:HG2	1:A:466:VAL:N	2.33	0.43
1:A:512:LYS:C	1:A:514:GLU:N	2.75	0.43
1:A:518:VAL:O	1:A:522:ILE:HG13	2.18	0.43
1:A:111:VAL:HG22	1:A:185:ASP:O	2.18	0.43
1:A:512:LYS:HA	1:A:519:ASN:CG	2.43	0.43
1:A:533:LEU:HA	1:A:533:LEU:HD23	1.80	0.43
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.18	0.43
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.54	0.43
1:A:331:LYS:HD2	1:A:364:ASP:OD1	2.19	0.43
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.53	0.43
2:B:7:THR:HG23	2:B:121:ASP:HA	2.00	0.43
2:B:60:VAL:HG12	2:B:75:VAL:HG22	2.00	0.43
1:A:241:VAL:O	1:A:242:GLN:C	2.62	0.43
1:A:308:GLU:HA	1:A:311:LYS:HG2	2.00	0.43
1:A:475:GLN:NE2	1:A:501:TYR:CZ	2.86	0.43
1:A:511:ASP:HA	1:A:522:ILE:HD13	2.01	0.43
2:B:314:VAL:CG2	2:B:315:HIS:N	2.81	0.43
1:A:291:GLU:O	1:A:293:ILE:HG13	2.19	0.43
2:B:112:GLY:CA	2:B:185:ASP:HB3	2.49	0.43
1:A:394:GLN:O	1:A:395:LYS:C	2.62	0.43
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.51	0.43
2:B:103:LYS:HA	2:B:103:LYS:HD3	1.79	0.43
2:B:360:ALA:O	2:B:361:HIS:CD2	2.72	0.43
2:B:393:ILE:HG12	2:B:394:GLN:N	2.33	0.43
1:A:206:ARG:HH21	1:A:216:THR:C	2.27	0.43
1:A:76:ASP:OD2	1:A:78:ARG:NH1	2.52	0.43
1:A:310:LEU:O	1:A:311:LYS:C	2.62	0.43
2:B:390:LYS:HB3	2:B:417:VAL:HG11	2.01	0.43
1:A:459:THR:HG22	1:A:463:ARG:CA	2.49	0.42
2:B:153:TRP:CE2	2:B:155:GLY:HA3	2.54	0.42
2:B:108:VAL:HB	2:B:232:TYR:HB3	2.01	0.42
2:B:279:LEU:CD2	2:B:282:LEU:HD12	2.48	0.42
1:A:296:THR:HG22	1:A:298:GLU:N	2.33	0.42
1:A:453:GLY:O	1:A:469:LEU:HB2	2.20	0.42
1:A:183:TYR:O	1:A:185:ASP:N	2.52	0.42
1:A:409:THR:OG1	1:A:410:TRP:N	2.52	0.42
2:B:92:LEU:O	2:B:93:GLY:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:GLU:O	2:B:197:GLN:N	2.52	0.42
1:A:306:ASN:O	1:A:310:LEU:HD13	2.19	0.42
1:A:364:ASP:HB2	1:A:424:LYS:HZ3	1.84	0.42
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.82	0.42
2:B:361:HIS:O	2:B:362:THR:OG1	2.30	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.55	0.42
1:A:395:LYS:HG3	1:A:414:TRP:CZ2	2.54	0.42
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.44	0.42
1:A:469:LEU:HD23	1:A:469:LEU:HA	1.86	0.42
2:B:20:LYS:HE2	2:B:55:PRO:HB2	2.00	0.42
2:B:84:THR:HG21	2:B:124:PHE:HZ	1.84	0.42
1:A:276:VAL:HG12	1:A:280:CYS:HB3	2.01	0.42
1:A:452:LEU:HD22	1:A:470:THR:HG22	2.01	0.42
1:A:479:LEU:O	1:A:521:ILE:HD11	2.20	0.42
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.55	0.42
2:B:70:LYS:HB2	2:B:70:LYS:HE3	1.85	0.42
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.55	0.42
2:B:139:THR:CB	2:B:140:PRO:HD2	2.41	0.42
2:B:401:TRP:O	2:B:402:TRP:C	2.62	0.42
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.55	0.41
1:A:501:TYR:CZ	1:A:505:ILE:CD1	3.03	0.41
2:B:371:ALA:O	2:B:375:ILE:HG13	2.18	0.41
1:A:175:ASN:OD1	1:A:201:LYS:NZ	2.45	0.41
1:A:276:VAL:O	1:A:277:ARG:C	2.62	0.41
2:B:278:GLN:CG	2:B:299:ALA:HA	2.51	0.41
1:A:283:LEU:O	1:A:284:ARG:C	2.64	0.41
1:A:379:SER:HA	1:A:383:TRP:CE3	2.55	0.41
2:B:8:VAL:O	2:B:9:PRO:C	2.63	0.41
1:A:23:GLN:HE22	1:A:60:VAL:H	1.68	0.41
1:A:208:HIS:NE2	1:A:212:TRP:NE1	2.63	0.41
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.43	0.41
1:A:535:TRP:CH2	2:B:422:LEU:HD11	2.56	0.41
2:B:254:VAL:HG23	2:B:291:GLU:O	2.21	0.41
1:A:407:GLN:HG2	2:B:393:ILE:HA	2.02	0.41
2:B:72:ARG:HH21	2:B:151:GLN:NE2	2.19	0.41
1:A:164:MET:HE1	1:A:168:LEU:HD11	2.03	0.41
2:B:126:LYS:HE2	2:B:127:TYR:OH	2.20	0.41
2:B:142:ILE:H	2:B:142:ILE:CD1	2.30	0.41
2:B:345:PRO:C	2:B:346:PHE:HD1	2.29	0.41
1:A:27:THR:CG2	1:A:29:GLU:HB3	2.51	0.41
1:A:126:LYS:C	1:A:128:THR:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:O	1:A:128:THR:N	2.54	0.41
1:A:182:GLN:O	1:A:183:TYR:CD1	2.74	0.41
1:A:394:GLN:O	1:A:397:THR:N	2.52	0.41
2:B:36:GLU:CG	2:B:37:ILE:N	2.84	0.41
2:B:183:TYR:CD2	2:B:184:MET:HB2	2.56	0.41
2:B:300:GLU:C	2:B:302:GLU:N	2.79	0.41
1:A:68:SER:O	1:A:69:THR:CG2	2.69	0.41
1:A:517:LEU:C	1:A:517:LEU:HD23	2.45	0.41
2:B:23:GLN:OE1	2:B:60:VAL:HG22	2.20	0.41
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.02	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD3	1.82	0.40
1:A:364:ASP:CB	1:A:424:LYS:HZ3	2.34	0.40
1:A:480:GLN:HG2	1:A:517:LEU:HD11	2.03	0.40
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.83	0.40
2:B:167:ILE:O	2:B:167:ILE:HG22	2.20	0.40
2:B:206:ARG:HE	2:B:217:PRO:HD2	1.86	0.40
2:B:278:GLN:HG2	2:B:302:GLU:HB2	2.02	0.40
2:B:328:GLU:HG2	2:B:390:LYS:CG	2.47	0.40
1:A:171:PHE:CE2	1:A:205:LEU:HA	2.57	0.40
2:B:129:ALA:HA	2:B:144:TYR:O	2.21	0.40
1:A:323:LYS:HE2	1:A:344:GLU:OE2	2.21	0.40
1:A:362:THR:O	1:A:510:PRO:HA	2.21	0.40
1:A:444:GLY:O	1:A:445:ALA:HB2	2.22	0.40
2:B:253:THR:O	2:B:257:ILE:HG13	2.21	0.40
1:A:20:LYS:O	1:A:21:VAL:C	2.65	0.40
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.51	0.40
2:B:90:VAL:O	2:B:91:GLN:C	2.63	0.40
2:B:107:THR:HA	2:B:232:TYR:O	2.21	0.40
2:B:299:ALA:O	2:B:302:GLU:N	2.55	0.40
1:A:276:VAL:O	1:A:276:VAL:CG1	2.69	0.40
2:B:253:THR:HA	2:B:292:VAL:HA	2.02	0.40
2:B:284:ARG:O	2:B:287:LYS:HD2	2.22	0.40
2:B:365:VAL:HG12	2:B:405:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/560 (95%)	442 (83%)	51 (10%)	38 (7%)	1	2
2	B	407/440 (92%)	334 (82%)	47 (12%)	26 (6%)	1	3
All	All	938/1000 (94%)	776 (83%)	98 (10%)	64 (7%)	1	2

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	137	ASN
1	A	141	GLY
1	A	225	PRO
1	A	230	MET
1	A	347	LYS
1	A	360	ALA
1	A	418	ASN
1	A	516	GLU
2	B	7	THR
2	B	93	GLY
2	B	214	LEU
2	B	241	VAL
2	B	313	PRO
2	B	358	ARG
1	A	14	PRO
1	A	85	GLN
1	A	237	ASP
1	A	346	PHE
1	A	426	TRP
1	A	443	ASP
2	B	9	PRO
2	B	285	GLY
2	B	345	PRO
2	B	361	HIS

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Mol	Chain	Res	Type
2	B	421	PRO
1	A	69	THR
1	A	91	GLN
1	A	193	LEU
1	A	195	ILE
1	A	269	GLN
1	A	289	LEU
1	A	295	LEU
1	A	311	LYS
1	A	361	HIS
1	A	412	PRO
2	B	14	PRO
2	B	195	ILE
2	B	217	PRO
2	B	272	PRO
2	B	286	THR
2	B	300	GLU
1	A	55	PRO
1	A	78	ARG
1	A	113	ASP
1	A	270	ILE
1	A	321	PRO
1	A	512	LYS
2	B	116	PHE
2	B	277	ARG
2	B	419	THR
1	A	122	GLU
2	B	98	ALA
2	B	176	PRO
2	B	193	LEU
1	A	90	VAL
1	A	276	VAL
2	B	298	GLU
1	A	510	PRO
1	A	537	PRO
2	B	317	VAL
1	A	21	VAL
1	A	433	PRO
2	B	247	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/500 (96%)	455 (95%)	25 (5%)	21	53
2	B	373/400 (93%)	351 (94%)	22 (6%)	18	48
All	All	853/900 (95%)	806 (94%)	47 (6%)	19	51

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	14	PRO
1	A	24	TRP
1	A	83	ARG
1	A	91	GLN
1	A	92	LEU
1	A	101	LYS
1	A	126	LYS
1	A	130	PHE
1	A	138	GLU
1	A	165	THR
1	A	177	ASP
1	A	188	TYR
1	A	216	THR
1	A	225	PRO
1	A	243	PRO
1	A	244	ILE
1	A	248	GLU
1	A	353	LYS
1	A	358	ARG
1	A	364	ASP
1	A	368	LEU
1	A	402	TRP
1	A	420	PRO
1	A	499	SER
2	B	9	PRO
2	B	40	GLU

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Mol	Chain	Res	Type
2	B	53	GLU
2	B	68	SER
2	B	95	PRO
2	B	118	VAL
2	B	126	LYS
2	B	151	GLN
2	B	156	SER
2	B	175	ASN
2	B	184	MET
2	B	187	LEU
2	B	216	THR
2	B	244	ILE
2	B	301	LEU
2	B	345	PRO
2	B	368	LEU
2	B	378	GLU
2	B	388	LYS
2	B	399	GLU
2	B	413	GLU
2	B	418	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	136	ASN
1	A	137	ASN
1	A	182	GLN
1	A	278	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	361	HIS
1	A	373	GLN
1	A	474	ASN
1	A	475	GLN
1	A	500	GLN
1	A	509	GLN
1	A	520	GLN
2	B	91	GLN
2	B	136	ASN
2	B	147	ASN

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Mol	Chain	Res	Type
2	B	151	GLN
2	B	197	GLN
2	B	278	GLN
2	B	361	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CP9	A	561	-	30,31,31	1.77	6 (20%)	41,45,45	1.49	6 (14%)

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	CP9	A	561	-	-	4/8/8/8	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	CP9	C14-N17	6.08	1.52	1.44
3	A	561	CP9	C2-N3	2.71	1.40	1.37
3	A	561	CP9	C22-C21	2.20	1.43	1.39
3	A	561	CP9	C13-C14	2.09	1.43	1.39
3	A	561	CP9	C9-C4	2.09	1.42	1.39
3	A	561	CP9	C21-N17	2.05	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	CP9	C21-N17-C18	-5.74	104.31	106.48
3	A	561	CP9	C11-C10-N3	3.12	118.54	113.46
3	A	561	CP9	C26-C18-N19	-2.94	121.07	124.80
3	A	561	CP9	C14-N17-C18	2.57	130.40	126.80
3	A	561	CP9	C22-C21-N17	2.26	134.65	130.54
3	A	561	CP9	C5-S1-C2	2.12	92.19	91.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	561	CP9	C13-C14-N17-C18
3	A	561	CP9	C13-C14-N17-C21
3	A	561	CP9	C15-C14-N17-C18
3	A	561	CP9	C15-C14-N17-C21

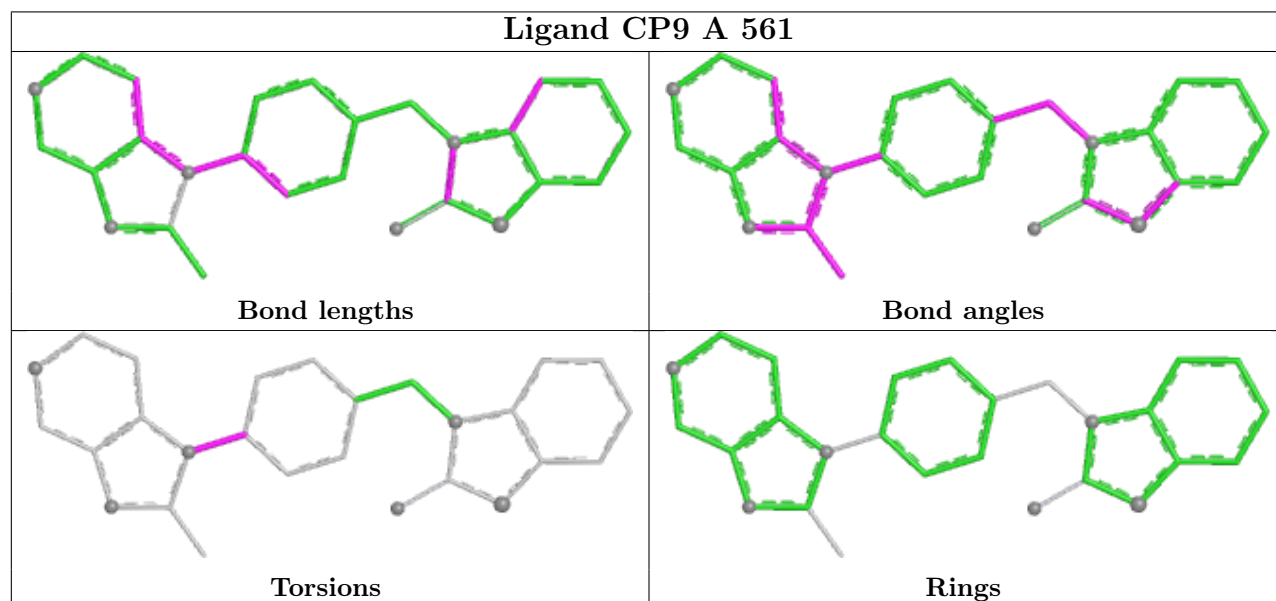
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	CP9	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	535/560 (95%)	1.09	99 (18%) 3 2	12, 59, 95, 107	0
2	B	411/440 (93%)	0.65	71 (17%) 4 3	4, 38, 99, 105	0
All	All	946/1000 (94%)	0.90	170 (17%) 3 3	4, 53, 98, 107	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	422	LEU	6.1
1	A	140	PRO	5.9
2	B	423	VAL	5.4
2	B	421	PRO	5.2
1	A	290	THR	5.1
2	B	357	MET	4.9
1	A	134	SER	4.5
1	A	183	TYR	4.4
1	A	37	ILE	4.4
1	A	225	PRO	4.1
2	B	283	LEU	4.1
2	B	231	GLY	4.1
2	B	215	THR	4.0
1	A	133	PRO	4.0
2	B	358	ARG	4.0
2	B	295	LEU	4.0
1	A	31	ILE	3.9
1	A	135	ILE	3.9
1	A	92	LEU	3.8
2	B	362	THR	3.8
1	A	444	GLY	3.7
1	A	21	VAL	3.7
1	A	474	ASN	3.7
2	B	312	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	63	ILE	3.7
1	A	22	LYS	3.6
1	A	32	LYS	3.6
1	A	24	TRP	3.5
2	B	266	TRP	3.5
1	A	358	ARG	3.5
1	A	65	LYS	3.4
1	A	313	PRO	3.3
1	A	129	ALA	3.3
2	B	426	TRP	3.3
2	B	216	THR	3.2
1	A	51	GLY	3.2
2	B	66	LYS	3.2
2	B	237	ASP	3.1
2	B	299	ALA	3.1
2	B	241	VAL	3.1
2	B	356	ARG	3.1
2	B	245	VAL	3.1
1	A	68	SER	3.1
1	A	25	PRO	3.1
2	B	272	PRO	3.1
1	A	110	ASP	3.1
1	A	137	ASN	3.1
2	B	285	GLY	3.1
2	B	296	THR	3.1
1	A	289	LEU	3.0
2	B	424	LYS	3.0
1	A	253	THR	3.0
2	B	316	GLY	3.0
1	A	33	ALA	3.0
2	B	239	TRP	2.9
1	A	510	PRO	2.9
2	B	292	VAL	2.9
2	B	195	ILE	2.9
1	A	426	TRP	2.9
2	B	247	PRO	2.9
1	A	288	ALA	2.9
2	B	242	GLN	2.8
2	B	8	VAL	2.8
2	B	284	ARG	2.8
1	A	34	LEU	2.8
2	B	294	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	235	HIS	2.8
1	A	139	THR	2.8
1	A	61	PHE	2.7
1	A	50	ILE	2.7
1	A	223	LYS	2.7
2	B	250	ASP	2.7
1	A	182	GLN	2.7
1	A	132	ILE	2.7
1	A	236	PRO	2.7
2	B	313	PRO	2.7
2	B	305	GLU	2.7
2	B	246	LEU	2.7
1	A	152	GLY	2.7
1	A	185	ASP	2.7
1	A	66	LYS	2.6
2	B	287	LYS	2.6
1	A	52	PRO	2.6
1	A	421	PRO	2.6
1	A	286	THR	2.6
1	A	424	LYS	2.6
2	B	286	THR	2.6
2	B	244	ILE	2.6
1	A	112	GLY	2.6
1	A	227	PHE	2.6
1	A	416	PHE	2.6
2	B	293	ILE	2.6
1	A	131	THR	2.5
1	A	251	SER	2.5
2	B	273	GLY	2.5
2	B	427	TYR	2.5
1	A	39	THR	2.5
2	B	428	GLN	2.5
2	B	310	LEU	2.5
2	B	86	ASP	2.5
1	A	26	LEU	2.5
1	A	419	THR	2.5
2	B	419	THR	2.5
2	B	217	PRO	2.4
2	B	418	ASN	2.4
1	A	228	LEU	2.4
1	A	360	ALA	2.4
2	B	67	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	314	VAL	2.4
1	A	271	TYR	2.4
1	A	315	HIS	2.4
1	A	244	ILE	2.4
1	A	515	SER	2.4
1	A	362	THR	2.4
1	A	217	PRO	2.4
1	A	446	ALA	2.3
1	A	252	TRP	2.3
1	A	232	TYR	2.3
2	B	65	LYS	2.3
2	B	173	LYS	2.3
1	A	113	ASP	2.3
1	A	230	MET	2.3
1	A	72	ARG	2.3
1	A	403	THR	2.3
1	A	203	GLU	2.2
2	B	288	ALA	2.2
1	A	234	LEU	2.2
2	B	218	ASP	2.2
2	B	315	HIS	2.2
1	A	425	LEU	2.2
2	B	214	LEU	2.2
1	A	142	ILE	2.2
1	A	38	CYS	2.2
2	B	95	PRO	2.2
2	B	301	LEU	2.2
1	A	35	VAL	2.2
1	A	247	PRO	2.2
1	A	195	ILE	2.2
1	A	69	THR	2.2
2	B	240	THR	2.2
2	B	6	GLU	2.2
2	B	204	GLU	2.2
1	A	332	GLN	2.1
1	A	443	ASP	2.1
1	A	58	THR	2.1
2	B	282	LEU	2.1
1	A	144	TYR	2.1
1	A	181	TYR	2.1
1	A	345	PRO	2.1
2	B	243	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	20	LYS	2.1
1	A	435	VAL	2.1
1	A	335	GLY	2.1
1	A	328	GLU	2.1
1	A	314	VAL	2.0
1	A	193	LEU	2.0
2	B	303	LEU	2.0
1	A	186	ASP	2.0
2	B	177	ASP	2.0
1	A	71	TRP	2.0
1	A	402	TRP	2.0
2	B	70	LYS	2.0
2	B	268	SER	2.0
1	A	1	PRO	2.0
1	A	246	LEU	2.0
1	A	285	GLY	2.0
2	B	359	GLY	2.0
2	B	360	ALA	2.0
1	A	344	GLU	2.0
2	B	318	TYR	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 oligosaccharides in this entry.

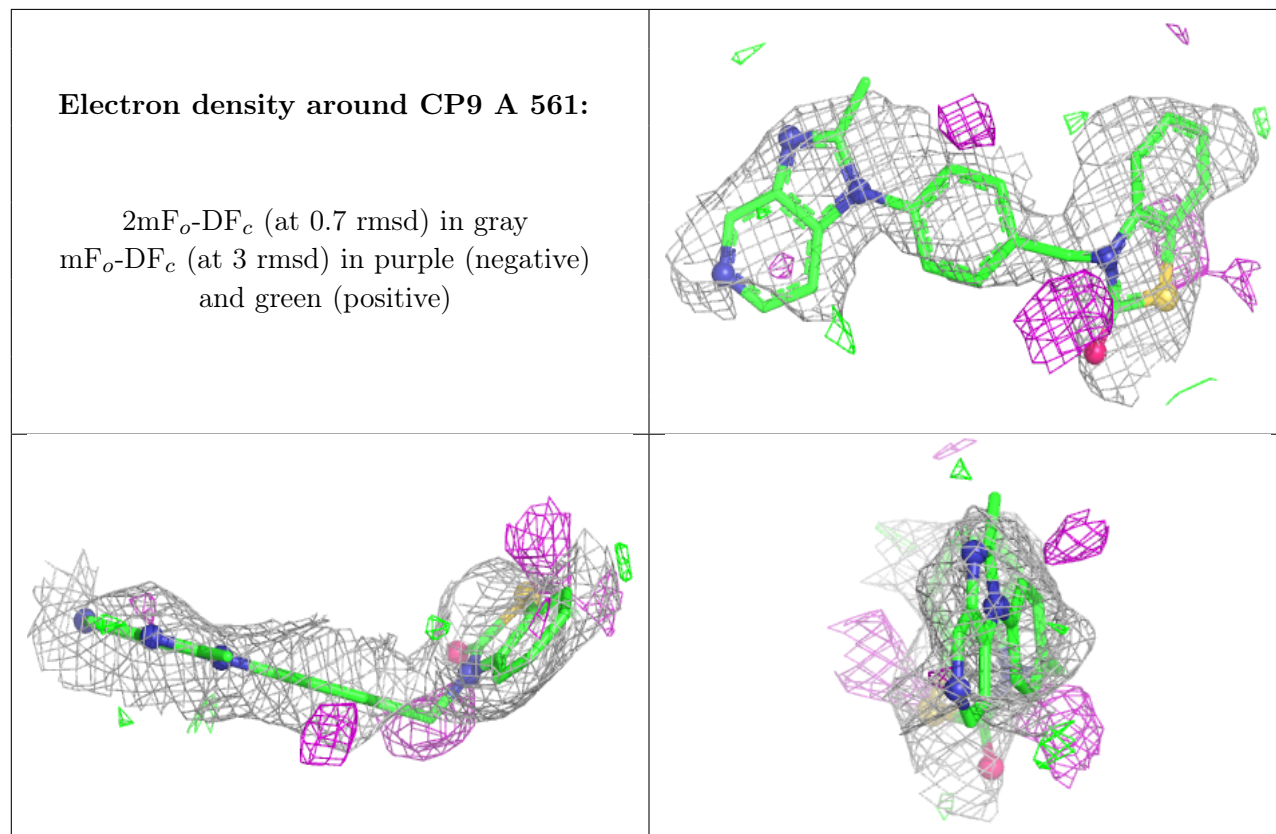
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CP9	A	561	27/27	0.73	0.20	62,68,73,74	0

The following is a graphical depiction of the model fit to experimental electron density of all

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



6.5 Other polymers [i](#)

There are no such residues in this entry.