



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:27 PM UTC

PDB ID : 3MEC / pdb_00003mec
Title : HIV-1 Reverse Transcriptase in Complex with TMC125
Authors : Lansdon, E.B.
Deposited on : 2010-03-31
Resolution : 2.30 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

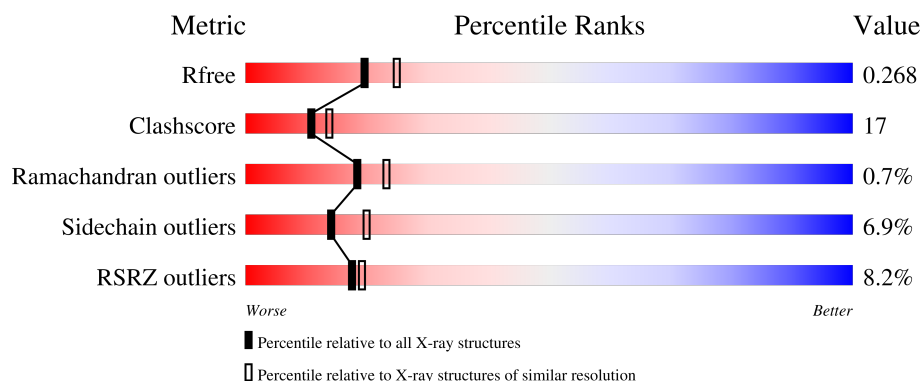
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

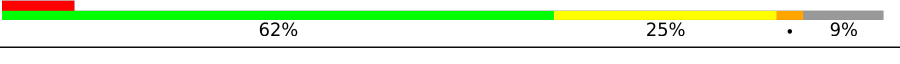
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 5 unique types of molecules in this entry. The entry contains 8072 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.

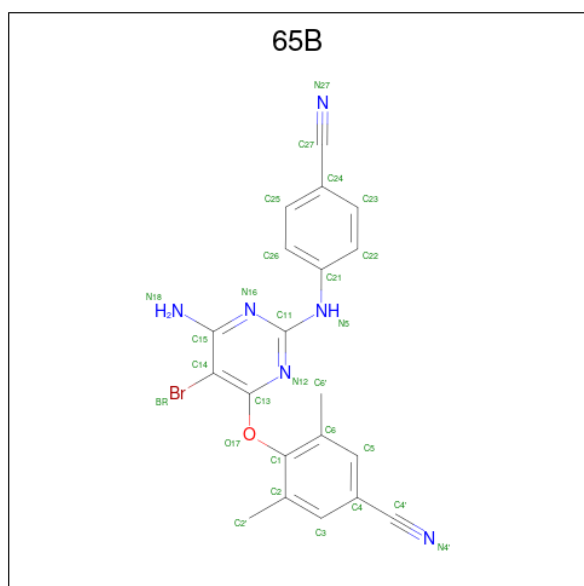
- Molecule 1 is a protein called p66 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4483	2900	746	829	8			

- Molecule 2 is a protein called p51 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3321	2164	548	603	6			

- Molecule 3 is 4-({6-AMINO-5-BROMO-2-[(4-CYANOPHENYL)AMINO]PYRIMIDIN-4-YL}OXY)-3,5-DIMETHYLBENZONITRILE (CCD ID: 65B) (formula: C₂₀H₁₅BrN₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			28	1	20	6	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

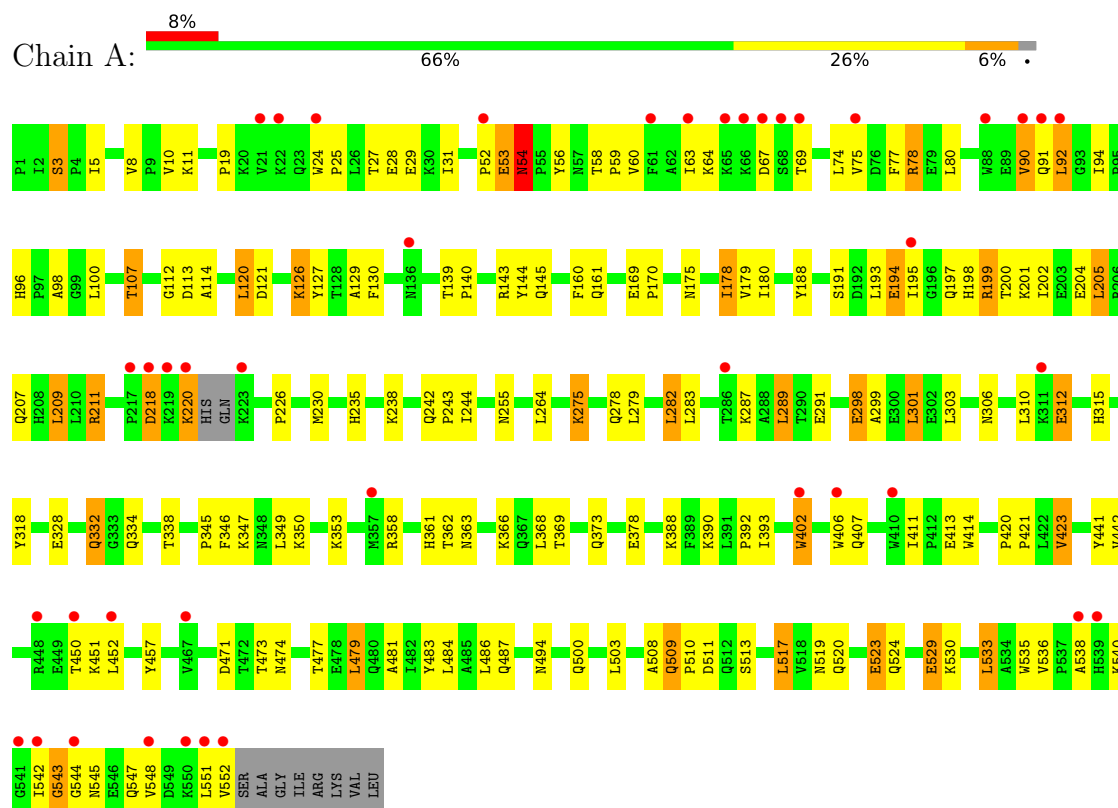
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	B	90	Total	O	0	0
			90	90		

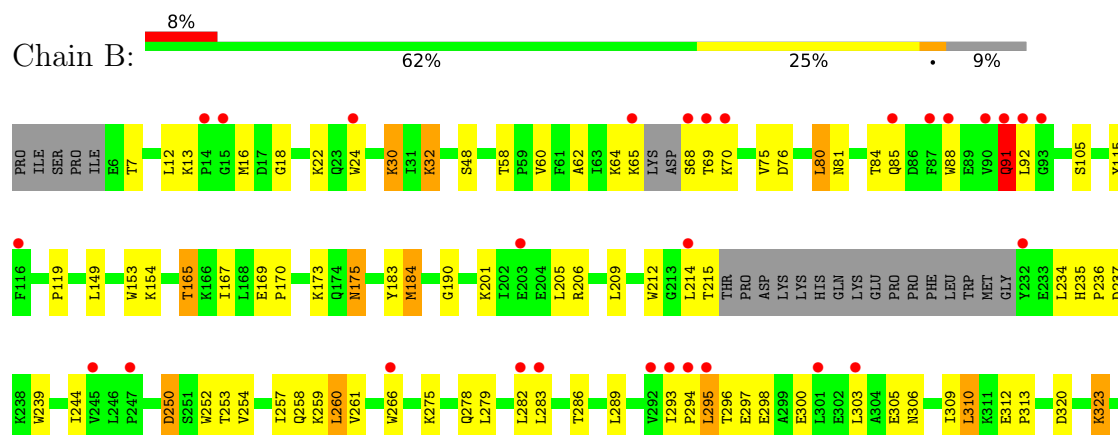
3 Residue-property plots [i](#)

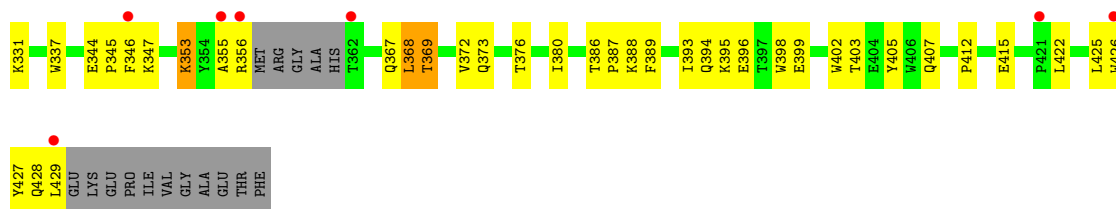
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 2: p51 Reverse transcriptase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.95Å 154.12Å 154.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.30 29.91 – 2.31	Depositor EDS
% Data completeness (in resolution range)	90.6 (29.91-2.30) 90.7 (29.91-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.32Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.226 , 0.270 0.224 , 0.268	Depositor DCC
R_{free} test set	2878 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8072	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: 65B, SO4

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	0/4598	0.75	4/6246 (0.1%)
2	B	0.40	0/3413	0.80	6/4637 (0.1%)
All	All	0.40	0/8011	0.77	10/10883 (0.1%)

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.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	18	GLY	CA-C-N	6.29	126.06	119.76
2	B	18	GLY	C-N-CA	6.29	126.06	119.76
1	A	54	ASN	CA-C-N	6.18	127.31	120.45
1	A	54	ASN	C-N-CA	6.18	127.31	120.45
1	A	3	SER	CA-C-N	5.97	126.75	120.12
1	A	3	SER	C-N-CA	5.97	126.75	120.12
2	B	235	HIS	CA-C-N	5.36	125.03	119.56
2	B	235	HIS	C-N-CA	5.36	125.03	119.56
2	B	175	ASN	CA-C-N	5.03	124.69	119.56
2	B	175	ASN	C-N-CA	5.03	124.69	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	91	GLN	Peptide

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	4483	0	4537	159	0
2	B	3321	0	3352	110	0
3	A	28	0	15	2	0
4	A	20	0	0	0	0
4	B	5	0	0	1	0
5	A	125	0	0	6	0
5	B	90	0	0	2	0
All	All	8072	0	7904	261	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 17.

All (261) 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:90:VAL:HG23	1:A:91:GLN:H	1.30	0.97
1:A:52:PRO:HA	1:A:53:GLU:C	1.95	0.92
2:B:260:LEU:HD13	2:B:279:LEU:HD21	1.53	0.87
1:A:92:LEU:HD23	1:A:92:LEU:H	1.44	0.82
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.62	0.82
1:A:194:GLU:CD	1:A:194:GLU:H	1.89	0.81
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.61	0.80
1:A:275:LYS:H	1:A:306:ASN:HD21	1.25	0.80
1:A:298:GLU:H	1:A:298:GLU:CD	1.93	0.77
1:A:520:GLN:O	1:A:523:GLU:HG3	1.87	0.75
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.68	0.75
2:B:296:THR:HG22	2:B:298:GLU:H	1.52	0.74
1:A:503:LEU:HD13	1:A:533:LEU:HD12	1.69	0.74
2:B:297:GLU:HG3	2:B:298:GLU:H	1.53	0.74
2:B:259:LYS:HE2	2:B:425:LEU:HD21	1.70	0.73
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.34	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.69	0.72
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.52	0.72
1:A:64:LYS:NZ	1:A:69:THR:HG22	2.05	0.72
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.73	0.71
1:A:96:HIS:HD1	1:A:98:ALA:H	1.39	0.70
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.73	0.70
2:B:69:THR:O	2:B:70:LYS:HG3	1.92	0.70
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.74	0.70
1:A:450:THR:HG22	1:A:452:LEU:HB2	1.73	0.69
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.08	0.69
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.22	0.69
2:B:81:ASN:ND2	2:B:154:LYS:H	1.91	0.68
2:B:13:LYS:HE3	2:B:16:MET:HE1	1.76	0.68
2:B:295:LEU:HD22	2:B:295:LEU:H	1.58	0.68
1:A:503:LEU:HD23	2:B:422:LEU:HD21	1.76	0.68
2:B:376:THR:HG23	2:B:386:THR:HG23	1.75	0.68
1:A:64:LYS:HZ3	1:A:69:THR:HA	1.60	0.67
1:A:191:SER:HB2	1:A:193:LEU:HD23	1.78	0.66
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.79	0.65
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.79	0.64
2:B:373:GLN:HE22	2:B:407:GLN:H	1.44	0.64
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.80	0.64
1:A:406:TRP:HE3	1:A:407:GLN:HE21	1.46	0.63
1:A:27:THR:HG22	1:A:29:GLU:H	1.62	0.63
1:A:486:LEU:HB3	1:A:524:GLN:HG3	1.81	0.63
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.33	0.63
1:A:90:VAL:HG23	1:A:91:GLN:N	2.09	0.63
1:A:175:ASN:HB3	1:A:178:ILE:CG2	2.29	0.62
2:B:373:GLN:NE2	2:B:407:GLN:H	1.97	0.62
1:A:169:GLU:HB2	1:A:170:PRO:HD3	1.82	0.62
2:B:297:GLU:HG3	2:B:298:GLU:N	2.15	0.61
1:A:64:LYS:HZ1	1:A:69:THR:HG22	1.63	0.61
1:A:334:GLN:HB3	5:A:611:HOH:O	1.99	0.61
2:B:91:GLN:HE21	2:B:91:GLN:C	2.09	0.61
1:A:509:GLN:N	1:A:510:PRO:HD3	2.16	0.61
1:A:175:ASN:HD22	1:A:201:LYS:NZ	1.99	0.60
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.02	0.60
2:B:293:ILE:HG13	2:B:294:PRO:HD2	1.82	0.60
1:A:175:ASN:ND2	1:A:201:LYS:NZ	2.49	0.60
1:A:197:GLN:O	1:A:201:LYS:HG2	2.02	0.60
2:B:13:LYS:HB2	2:B:16:MET:SD	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:H	1:A:312:GLU:CD	2.09	0.60
2:B:295:LEU:HD22	2:B:295:LEU:N	2.17	0.59
1:A:120:LEU:HD22	1:A:121:ASP:H	1.66	0.59
1:A:242:GLN:O	1:A:244:ILE:HD12	2.02	0.59
2:B:32:LYS:NZ	2:B:32:LYS:HB2	2.17	0.59
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.12	0.59
1:A:54:ASN:ND2	1:A:56:TYR:H	2.01	0.59
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.38	0.59
1:A:287:LYS:HE3	1:A:291:GLU:OE2	2.02	0.59
2:B:81:ASN:HD21	2:B:154:LYS:H	1.50	0.58
2:B:275:LYS:H	2:B:306:ASN:HD21	1.51	0.58
2:B:393:ILE:HG12	2:B:394:GLN:N	2.19	0.58
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.68	0.58
1:A:175:ASN:HD22	1:A:201:LYS:HZ1	1.51	0.58
2:B:296:THR:HG22	2:B:298:GLU:N	2.19	0.57
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.39	0.57
2:B:80:LEU:HD22	2:B:84:THR:HG23	1.87	0.57
1:A:230:MET:HA	1:A:230:MET:HE2	1.86	0.57
2:B:393:ILE:HG12	2:B:394:GLN:H	1.69	0.57
2:B:184:MET:HE2	5:B:498:HOH:O	2.05	0.56
1:A:362:THR:HG22	1:A:366:LYS:HD2	1.87	0.56
2:B:12:LEU:HD23	2:B:84:THR:HG22	1.87	0.56
2:B:81:ASN:HD21	2:B:153:TRP:HA	1.70	0.56
1:A:195:ILE:O	1:A:199:ARG:HG3	2.06	0.56
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.88	0.56
1:A:19:PRO:HG3	1:A:80:LEU:HA	1.88	0.55
2:B:345:PRO:O	2:B:346:PHE:HB2	2.04	0.55
1:A:483:TYR:O	1:A:487:GLN:HG2	2.06	0.55
2:B:305:GLU:O	2:B:309:ILE:HG13	2.06	0.55
2:B:206:ARG:CZ	2:B:206:ARG:HB3	2.37	0.55
1:A:278:GLN:HG3	1:A:298:GLU:HB2	1.89	0.55
1:A:129:ALA:HA	1:A:144:TYR:O	2.06	0.55
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.88	0.55
2:B:259:LYS:NZ	2:B:425:LEU:HD11	2.23	0.54
1:A:52:PRO:CA	1:A:53:GLU:C	2.77	0.54
1:A:420:PRO:HA	1:A:421:PRO:C	2.32	0.54
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.38	0.54
1:A:120:LEU:HD22	1:A:121:ASP:N	2.21	0.54
1:A:368:LEU:HD22	1:A:423:VAL:HG11	1.90	0.54
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.88	0.54
2:B:282:LEU:HB3	2:B:293:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.88	0.54
1:A:92:LEU:H	1:A:92:LEU:CD2	2.17	0.54
1:A:350:LYS:HE3	1:A:378:GLU:OE2	2.08	0.53
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.43	0.53
1:A:503:LEU:CD1	1:A:533:LEU:HD12	2.35	0.53
1:A:536:VAL:HG13	1:A:542:ILE:HG13	1.89	0.53
1:A:24:TRP:CD2	1:A:25:PRO:HD2	2.44	0.53
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.91	0.53
1:A:178:ILE:C	1:A:178:ILE:HD13	2.34	0.52
1:A:175:ASN:ND2	1:A:201:LYS:HZ1	2.06	0.52
1:A:393:ILE:CB	1:A:423:VAL:HG13	2.40	0.52
1:A:27:THR:CG2	1:A:29:GLU:HG2	2.39	0.52
1:A:27:THR:HG21	5:A:610:HOH:O	2.09	0.52
2:B:253:THR:O	2:B:257:ILE:HG12	2.09	0.52
1:A:205:LEU:HD22	1:A:209:LEU:HD22	1.92	0.52
2:B:237:ASP:C	2:B:239:TRP:H	2.18	0.52
1:A:27:THR:O	1:A:31:ILE:HG13	2.10	0.52
1:A:107:THR:HG22	1:A:198:HIS:NE2	2.24	0.52
2:B:395:LYS:O	2:B:399:GLU:HG3	2.10	0.52
2:B:425:LEU:HD12	2:B:428:GLN:OE1	2.09	0.52
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.26	0.51
1:A:200:THR:O	1:A:204:GLU:HG3	2.10	0.51
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.92	0.51
1:A:369:THR:O	1:A:373:GLN:HG2	2.09	0.51
2:B:65:LYS:HB2	2:B:68:SER:HB2	1.92	0.51
1:A:53:GLU:O	1:A:54:ASN:C	2.54	0.51
1:A:402:TRP:CD1	2:B:331:LYS:HZ1	2.29	0.51
1:A:27:THR:HG21	1:A:29:GLU:HG2	1.92	0.51
1:A:107:THR:HG21	1:A:202:ILE:HG13	1.91	0.51
1:A:8:VAL:O	1:A:10:VAL:HG23	2.10	0.51
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.76	0.51
1:A:542:ILE:HD11	2:B:261:VAL:HG11	1.92	0.50
1:A:500:GLN:NE2	2:B:422:LEU:HD23	2.27	0.50
1:A:90:VAL:CG2	1:A:91:GLN:H	2.13	0.50
1:A:393:ILE:HG13	1:A:423:VAL:HG13	1.92	0.50
1:A:450:THR:O	1:A:451:LYS:HB2	2.12	0.50
2:B:306:ASN:O	2:B:310:LEU:HD22	2.11	0.50
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.10	0.50
2:B:214:LEU:HD13	2:B:214:LEU:C	2.37	0.50
1:A:298:GLU:CD	1:A:298:GLU:N	2.68	0.49
1:A:529:GLU:O	1:A:530:LYS:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:C	1:A:54:ASN:HD22	2.20	0.49
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.47	0.49
2:B:30:LYS:HE3	2:B:403:THR:HG21	1.93	0.49
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.28	0.49
1:A:547:GLN:O	1:A:551:LEU:HD13	2.13	0.49
2:B:64:LYS:O	2:B:65:LYS:C	2.56	0.49
2:B:394:GLN:NE2	2:B:396:GLU:HB2	2.27	0.49
1:A:126:LYS:HA	1:A:145:GLN:NE2	2.28	0.49
2:B:214:LEU:HD13	2:B:214:LEU:O	2.12	0.49
1:A:52:PRO:HA	1:A:54:ASN:N	2.27	0.48
1:A:178:ILE:HG12	1:A:179:VAL:N	2.27	0.48
1:A:451:LYS:HD2	1:A:451:LYS:N	2.28	0.48
2:B:165:THR:HG22	5:B:459:HOH:O	2.12	0.48
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.48	0.48
2:B:296:THR:O	2:B:300:GLU:HG2	2.13	0.48
2:B:24:TRP:CZ3	2:B:399:GLU:HB3	2.48	0.48
2:B:355:ALA:O	2:B:356:ARG:HB3	2.13	0.48
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.49	0.48
2:B:24:TRP:CD1	2:B:24:TRP:N	2.81	0.48
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.49	0.48
1:A:191:SER:HB2	1:A:193:LEU:CD2	2.42	0.48
2:B:24:TRP:CD1	2:B:24:TRP:H	2.32	0.47
2:B:376:THR:O	2:B:380:ILE:HG13	2.14	0.47
1:A:450:THR:CG2	1:A:452:LEU:HB2	2.41	0.47
2:B:394:GLN:HE21	2:B:396:GLU:HB2	1.78	0.47
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.29	0.47
1:A:126:LYS:HD2	5:A:652:HOH:O	2.15	0.47
1:A:393:ILE:CG1	1:A:423:VAL:HG13	2.45	0.47
2:B:154:LYS:HG2	2:B:184:MET:CE	2.45	0.47
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.97	0.47
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.74	0.47
2:B:58:THR:HG23	2:B:76:ASP:O	2.15	0.47
2:B:169:GLU:OE1	2:B:173:LYS:HE3	2.15	0.47
1:A:92:LEU:CD1	2:B:22:LYS:HE2	2.44	0.46
1:A:191:SER:CB	1:A:193:LEU:HD23	2.45	0.46
2:B:388:LYS:HE2	2:B:415:GLU:OE1	2.14	0.46
2:B:30:LYS:HE3	2:B:403:THR:CG2	2.44	0.46
1:A:457:TYR:HA	1:A:548:VAL:HG21	1.96	0.46
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.51	0.46
1:A:349:LEU:HD12	1:A:349:LEU:N	2.30	0.46
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:PRO:O	1:A:423:VAL:HG12	2.15	0.46
1:A:27:THR:HG22	1:A:29:GLU:N	2.29	0.46
1:A:92:LEU:HD12	2:B:22:LYS:HE2	1.98	0.46
2:B:398:TRP:O	2:B:402:TRP:HD1	1.99	0.46
1:A:220:LYS:HD2	1:A:220:LYS:HA	1.62	0.46
1:A:538:ALA:HA	1:A:545:ASN:HD21	1.81	0.46
1:A:77:PHE:O	1:A:78:ARG:C	2.58	0.45
2:B:69:THR:C	2:B:70:LYS:HG3	2.40	0.45
2:B:80:LEU:HD13	2:B:153:TRP:CD1	2.51	0.45
2:B:239:TRP:NE1	4:B:441:SO4:O4	2.47	0.45
2:B:320:ASP:OD2	2:B:323:LYS:HD3	2.16	0.45
1:A:406:TRP:CE3	1:A:407:GLN:NE2	2.85	0.45
1:A:345:PRO:HA	1:A:346:PHE:HA	1.53	0.45
1:A:513:SER:H	1:A:519:ASN:HD21	1.64	0.45
2:B:282:LEU:HB3	2:B:293:ILE:CD1	2.45	0.45
2:B:175:ASN:HD21	2:B:201:LYS:HZ2	1.65	0.45
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.99	0.45
2:B:237:ASP:C	2:B:239:TRP:N	2.74	0.45
1:A:524:GLN:NE2	5:A:589:HOH:O	2.50	0.45
2:B:254:VAL:O	2:B:258:GLN:HG3	2.16	0.45
2:B:422:LEU:N	2:B:422:LEU:HD22	2.32	0.45
1:A:358:ARG:NH1	2:B:394:GLN:HG3	2.33	0.44
2:B:278:GLN:NE2	2:B:298:GLU:HB3	2.32	0.44
1:A:169:GLU:CB	1:A:170:PRO:HD3	2.46	0.44
1:A:332:GLN:NE2	1:A:338:THR:HG21	2.33	0.44
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.52	0.44
1:A:54:ASN:HD22	1:A:56:TYR:H	1.66	0.44
1:A:536:VAL:CG1	1:A:542:ILE:HG13	2.46	0.44
2:B:320:ASP:OD1	2:B:320:ASP:C	2.61	0.44
1:A:100:LEU:O	1:A:318:TYR:HB3	2.18	0.44
1:A:484:LEU:HA	1:A:484:LEU:HD23	1.81	0.44
2:B:259:LYS:HZ1	2:B:425:LEU:HD11	1.81	0.44
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.53	0.44
1:A:363:ASN:HA	1:A:511:ASP:CG	2.42	0.44
1:A:411:ILE:HG13	1:A:414:TRP:CD1	2.53	0.44
1:A:53:GLU:H	1:A:53:GLU:CD	2.26	0.43
1:A:287:LYS:HG3	1:A:291:GLU:CD	2.43	0.43
3:A:561:65B:H26	3:A:561:65B:N12	2.33	0.43
1:A:194:GLU:CD	1:A:194:GLU:N	2.67	0.43
2:B:353:LYS:HD2	2:B:353:LYS:C	2.43	0.43
2:B:368:LEU:O	2:B:372:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LYS:HB2	2:B:32:LYS:HZ3	1.83	0.43
1:A:538:ALA:HA	1:A:545:ASN:ND2	2.33	0.43
1:A:126:LYS:HG2	1:A:127:TYR:N	2.34	0.42
2:B:13:LYS:HE3	2:B:16:MET:CE	2.46	0.42
1:A:178:ILE:HD11	1:A:180:ILE:HG13	2.00	0.42
1:A:279:LEU:O	1:A:282:LEU:HB2	2.18	0.42
2:B:386:THR:CG2	2:B:412:PRO:HB3	2.49	0.42
2:B:303:LEU:HD23	2:B:303:LEU:N	2.35	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
1:A:211:ARG:NH2	5:A:572:HOH:O	2.52	0.42
2:B:91:GLN:C	2:B:91:GLN:NE2	2.76	0.42
2:B:214:LEU:HD13	2:B:215:THR:O	2.20	0.42
1:A:96:HIS:CE1	1:A:350:LYS:HD2	2.55	0.42
1:A:542:ILE:O	1:A:543:GLY:C	2.62	0.42
1:A:242:GLN:HB2	1:A:243:PRO:HD2	2.02	0.42
1:A:312:GLU:CD	1:A:312:GLU:N	2.75	0.42
2:B:405:TYR:O	2:B:407:GLN:HG3	2.20	0.42
1:A:188:TYR:HB3	3:A:561:65B:C3	2.49	0.41
1:A:413:GLU:HA	5:A:605:HOH:O	2.20	0.41
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.49	0.41
1:A:508:ALA:O	1:A:509:GLN:HB3	2.20	0.41
2:B:422:LEU:HB3	2:B:426:TRP:CH2	2.55	0.41
2:B:266:TRP:CH2	2:B:427:TYR:CZ	3.08	0.41
2:B:30:LYS:HD2	2:B:62:ALA:HB3	2.02	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.41
2:B:373:GLN:HE22	2:B:407:GLN:N	2.15	0.41
1:A:3:SER:OG	1:A:5:ILE:HG22	2.20	0.41
2:B:244:ILE:HG12	2:B:266:TRP:HZ3	1.85	0.41
1:A:548:VAL:O	1:A:552:VAL:HG22	2.21	0.41
2:B:24:TRP:H	2:B:24:TRP:HD1	1.69	0.41
2:B:154:LYS:CG	2:B:184:MET:HE1	2.50	0.41
1:A:27:THR:CG2	1:A:28:GLU:N	2.82	0.41
1:A:63:ILE:HD11	1:A:74:LEU:HD12	2.03	0.41
1:A:473:THR:O	1:A:477:THR:HG23	2.21	0.41
1:A:194:GLU:O	1:A:195:ILE:C	2.64	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.83	0.41
1:A:538:ALA:C	1:A:540:LYS:H	2.29	0.41
1:A:139:THR:HB	1:A:140:PRO:HD2	2.02	0.40
1:A:112:GLY:O	1:A:113:ASP:C	2.63	0.40
1:A:388:LYS:HB3	1:A:388:LYS:HE2	1.83	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	546/560 (98%)	511 (94%)	29 (5%)	6 (1%)	11	13
2	B	393/440 (89%)	378 (96%)	14 (4%)	1 (0%)	36	46
All	All	939/1000 (94%)	889 (95%)	43 (5%)	7 (1%)	18	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	90	VAL
1	A	218	ASP
2	B	250	ASP
1	A	543	GLY
1	A	78	ARG
1	A	509	GLN

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	492/500 (98%)	453 (92%)	39 (8%)	11	15
2	B	366/400 (92%)	346 (94%)	20 (6%)	19	28
All	All	858/900 (95%)	799 (93%)	59 (7%)	14	20

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	54	ASN
1	A	67	ASP
1	A	92	LEU
1	A	94	ILE
1	A	107	THR
1	A	120	LEU
1	A	126	LYS
1	A	161	GLN
1	A	178	ILE
1	A	194	GLU
1	A	199	ARG
1	A	205	LEU
1	A	209	LEU
1	A	211	ARG
1	A	218	ASP
1	A	220	LYS
1	A	264	LEU
1	A	275	LYS
1	A	282	LEU
1	A	283	LEU
1	A	289	LEU
1	A	298	GLU
1	A	301	LEU
1	A	303	LEU
1	A	310	LEU
1	A	312	GLU
1	A	332	GLN
1	A	347	LYS
1	A	353	LYS
1	A	361	HIS
1	A	402	TRP
1	A	423	VAL
1	A	474	ASN
1	A	479	LEU
1	A	517	LEU
1	A	523	GLU
1	A	529	GLU
1	A	533	LEU
2	B	30	LYS
2	B	32	LYS
2	B	48	SER
2	B	80	LEU

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Mol	Chain	Res	Type
2	B	91	GLN
2	B	92	LEU
2	B	165	THR
2	B	184	MET
2	B	205	LEU
2	B	209	LEU
2	B	234	LEU
2	B	250	ASP
2	B	260	LEU
2	B	295	LEU
2	B	310	LEU
2	B	323	LYS
2	B	353	LYS
2	B	368	LEU
2	B	369	THR
2	B	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	57	ASN
1	A	91	GLN
1	A	145	GLN
1	A	174	GLN
1	A	175	ASN
1	A	207	GLN
1	A	258	GLN
1	A	269	GLN
1	A	278	GLN
1	A	306	ASN
1	A	332	GLN
1	A	407	GLN
1	A	418	ASN
1	A	475	GLN
1	A	500	GLN
1	A	509	GLN
1	A	512	GLN
1	A	519	ASN
1	A	520	GLN
1	A	545	ASN
2	B	81	ASN

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Mol	Chain	Res	Type
2	B	85	GLN
2	B	91	GLN
2	B	151	GLN
2	B	175	ASN
2	B	255	ASN
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	336	GLN
2	B	348	ASN
2	B	367	GLN
2	B	373	GLN
2	B	394	GLN
2	B	407	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 oligosaccharides 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
3	65B	A	561	-	30,30,30	2.75	15 (50%)	40,42,42	1.71	5 (12%)
4	SO4	A	565	-	4,4,4	0.37	0	6,6,6	0.12	0
4	SO4	A	562	-	4,4,4	0.36	0	6,6,6	0.14	0
4	SO4	A	564	-	4,4,4	0.34	0	6,6,6	0.10	0
4	SO4	B	441	-	4,4,4	0.58	0	6,6,6	0.36	0
4	SO4	A	563	-	4,4,4	0.36	0	6,6,6	0.11	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	65B	A	561	-	-	0/12/12/12	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	65B	C13-N12	6.25	1.41	1.32
3	A	561	65B	C15-N16	5.85	1.42	1.35
3	A	561	65B	C26-C21	5.19	1.48	1.39
3	A	561	65B	C1-C6	3.85	1.46	1.40
3	A	561	65B	C1-C2	3.71	1.46	1.40
3	A	561	65B	C26-C25	3.67	1.44	1.38
3	A	561	65B	C5-C6	3.15	1.43	1.39
3	A	561	65B	C3-C2	2.98	1.43	1.39
3	A	561	65B	C11-N16	2.76	1.42	1.34
3	A	561	65B	C22-C21	2.56	1.43	1.39
3	A	561	65B	C23-C22	2.50	1.42	1.38
3	A	561	65B	C25-C24	2.38	1.44	1.39
3	A	561	65B	C23-C24	2.37	1.44	1.39
3	A	561	65B	C6'-C6	2.23	1.55	1.51
3	A	561	65B	C5-C4	2.19	1.43	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	65B	C11-N16-C15	5.12	120.74	116.59
3	A	561	65B	N16-C11-N12	-5.00	118.06	126.26
3	A	561	65B	C11-N12-C13	4.00	122.27	115.38
3	A	561	65B	C14-C13-N12	-3.02	120.53	123.78
3	A	561	65B	O17-C13-C14	2.90	119.76	117.89

There are no chirality outliers.

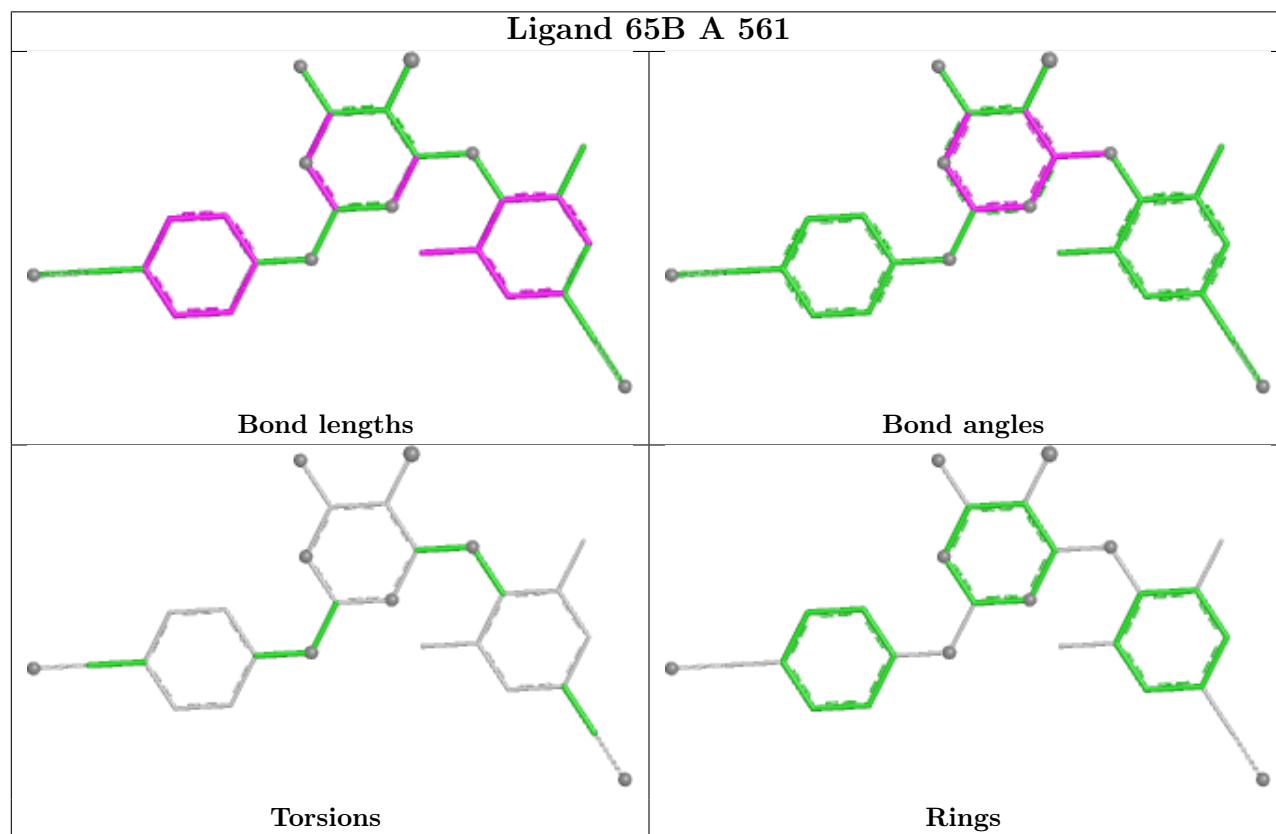
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	65B	2	0
4	B	441	SO4	1	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	550/560 (98%)	0.48	42 (7%)	20 21	30, 50, 90, 122	0
2	B	401/440 (91%)	0.46	36 (8%)	15 16	27, 49, 88, 104	0
All	All	951/1000 (95%)	0.47	78 (8%)	17 19	27, 50, 89, 122	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	551	LEU	5.6
2	B	92	LEU	5.1
2	B	87	PHE	4.4
1	A	286	THR	4.3
1	A	217	PRO	4.2
1	A	552	VAL	4.1
2	B	362	THR	4.0
2	B	295	LEU	4.0
1	A	548	VAL	3.9
1	A	92	LEU	3.9
1	A	24	TRP	3.9
1	A	220	LYS	3.8
1	A	357	MET	3.7
2	B	88	TRP	3.6
2	B	116	PHE	3.5
2	B	24	TRP	3.4
2	B	426	TRP	3.4
1	A	406	TRP	3.4
2	B	266	TRP	3.4
1	A	52	PRO	3.3
2	B	93	GLY	3.0
1	A	550	LYS	3.0
2	B	429	LEU	2.9
2	B	69	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	218	ASP	2.9
2	B	70	LYS	2.8
2	B	293	ILE	2.8
2	B	90	VAL	2.8
1	A	88	TRP	2.8
2	B	15	GLY	2.8
2	B	294	PRO	2.8
1	A	538	ALA	2.7
2	B	203	GLU	2.7
1	A	402	TRP	2.7
1	A	223	LYS	2.7
2	B	214	LEU	2.7
1	A	61	PHE	2.6
1	A	68	SER	2.6
1	A	66	LYS	2.6
1	A	219	LYS	2.6
1	A	90	VAL	2.6
2	B	245	VAL	2.6
2	B	282	LEU	2.6
1	A	69	THR	2.6
1	A	541	GLY	2.6
1	A	195	ILE	2.6
1	A	65	LYS	2.6
1	A	67	ASP	2.5
1	A	450	THR	2.5
1	A	63	ILE	2.4
2	B	232	TYR	2.4
1	A	452	LEU	2.4
2	B	65	LYS	2.4
2	B	283	LEU	2.4
2	B	346	PHE	2.3
2	B	14	PRO	2.3
2	B	303	LEU	2.3
1	A	539	HIS	2.3
2	B	355	ALA	2.3
1	A	22	LYS	2.3
1	A	410	TRP	2.2
2	B	301	LEU	2.2
2	B	356	ARG	2.2
2	B	247	PRO	2.2
1	A	467	VAL	2.2
1	A	91	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	85	GLN	2.1
2	B	91	GLN	2.1
1	A	311	LYS	2.1
1	A	136	ASN	2.1
1	A	542	ILE	2.1
1	A	75	VAL	2.1
2	B	292	VAL	2.1
2	B	421	PRO	2.1
1	A	544	GLY	2.1
2	B	68	SER	2.0
1	A	21	VAL	2.0
1	A	448	ARG	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](#)

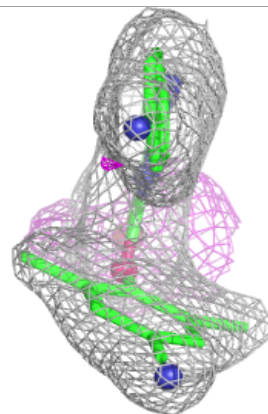
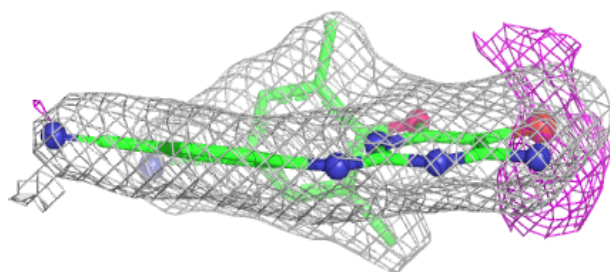
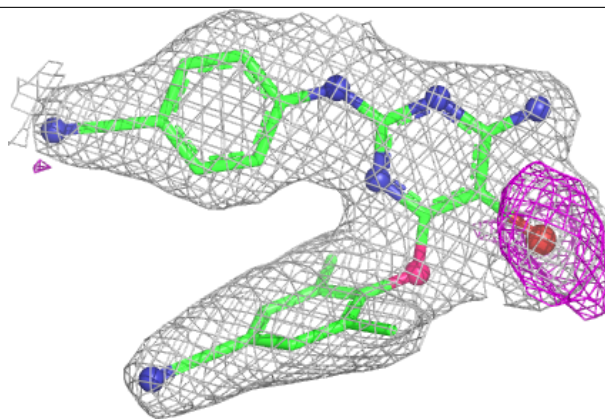
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	564	5/5	0.67	0.26	138,138,139,139	0
4	SO4	A	565	5/5	0.81	0.12	105,106,106,106	0
4	SO4	A	563	5/5	0.86	0.13	73,75,76,76	0
4	SO4	A	562	5/5	0.87	0.14	71,72,73,74	0
4	SO4	B	441	5/5	0.88	0.12	96,96,97,97	0
3	65B	A	561	28/28	0.92	0.10	35,38,42,70	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 65B 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.