



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2026 – 08:02 AM EDT

PDB ID : 3M8P / pdb_00003m8p
Title : HIV-1 RT with NNRTI TMC-125
Authors : Harris, S.F.; Villasenor, A.
Deposited on : 2010-03-18
Resolution : 2.67 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

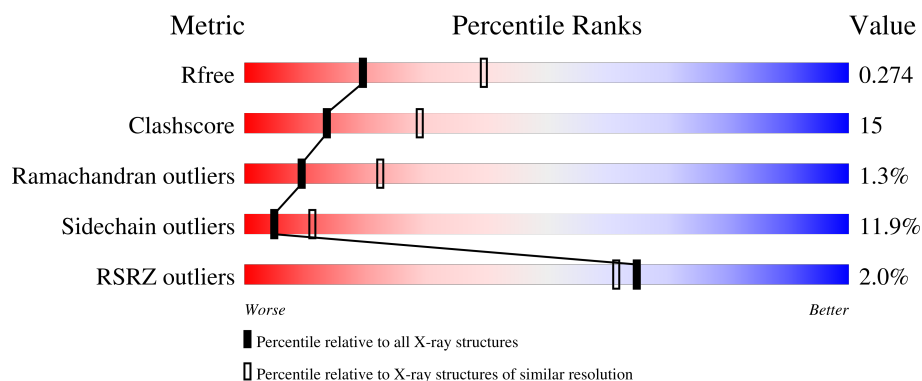
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

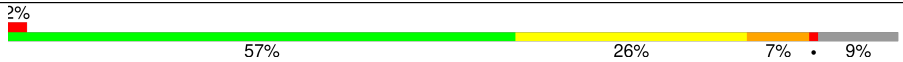
The reported resolution of this entry is 2.67 Å.

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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	561	
2	B	440	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8138 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

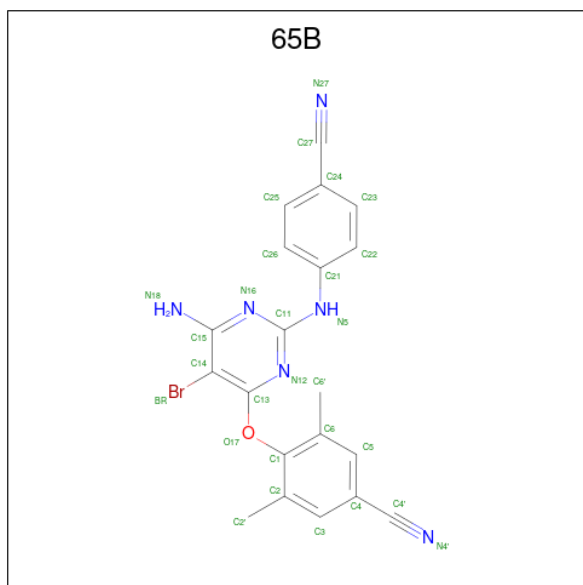
- Molecule 1 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4485	2900	748	829	8			

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3320	2166	545	602	7			

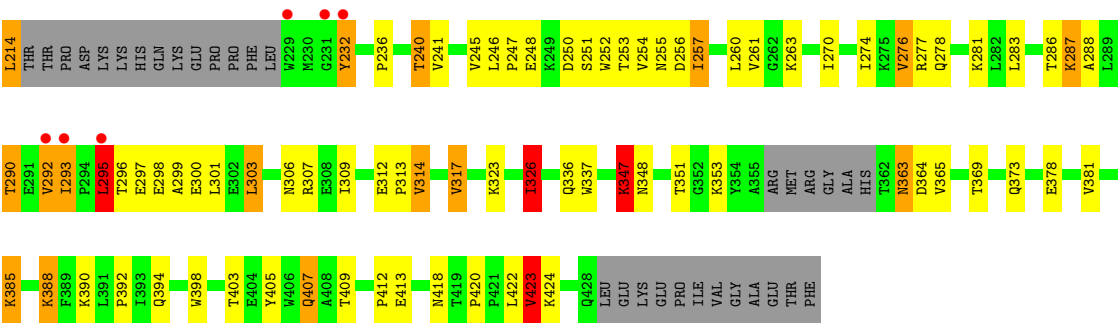
- Molecule 3 is Etravirine (CCD ID: 65B) (formula: C₂₀H₁₅BrN₆O).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total 169	O 169	0	0
4	B	136	Total 136	O 136	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.44Å 153.53Å 154.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.01 – 2.67 47.01 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.01-2.67) 99.7 (47.01-2.67)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.209 , 0.283 0.208 , 0.274	Depositor DCC
R_{free} test set	2042 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8138	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 65B

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	1.56	31/4601 (0.7%)	1.37	34/6252 (0.5%)
2	B	1.56	25/3414 (0.7%)	1.34	25/4640 (0.5%)
All	All	1.56	56/8015 (0.7%)	1.36	59/10892 (0.5%)

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	232	TYR	CA-C	13.47	1.58	1.52
1	A	420	PRO	CA-C	-10.05	1.45	1.52
1	A	409	THR	CA-CB	9.78	1.73	1.53
1	A	224	GLU	CA-C	7.53	1.59	1.52
2	B	412	PRO	N-CA	-7.14	1.39	1.47
1	A	180	ILE	C-O	-7.14	1.16	1.24
1	A	90	VAL	CA-CB	6.86	1.63	1.54
1	A	340	GLN	CA-C	-6.66	1.44	1.52
1	A	534	ALA	CA-CB	-6.63	1.40	1.54
2	B	21	VAL	C-O	-6.55	1.17	1.24
2	B	132	ILE	CA-CB	-6.50	1.45	1.54
2	B	240	THR	CA-CB	6.39	1.62	1.53
2	B	378	GLU	CA-C	-6.27	1.44	1.52
2	B	295	LEU	CA-C	6.25	1.60	1.52
2	B	139	THR	CB-CG2	6.24	1.73	1.52
2	B	114	ALA	CA-CB	-6.18	1.43	1.53
1	A	505	ILE	CA-CB	-6.17	1.47	1.54
2	B	13	LYS	CA-C	6.07	1.60	1.52
1	A	161	GLN	CA-C	-6.01	1.44	1.52
2	B	326	ILE	CA-CB	6.00	1.64	1.55
2	B	32	LYS	CA-C	-5.91	1.45	1.52
1	A	338	THR	C-O	-5.78	1.16	1.23
1	A	8	VAL	C-O	-5.74	1.18	1.24
1	A	484	LEU	C-O	-5.66	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	190	GLY	CA-C	5.61	1.56	1.52
2	B	392	PRO	CA-C	-5.61	1.48	1.53
1	A	106	VAL	CA-CB	5.59	1.64	1.55
1	A	125	ARG	CA-C	-5.59	1.45	1.52
1	A	318	TYR	C-O	-5.58	1.16	1.23
1	A	286	THR	CA-CB	5.56	1.59	1.53
2	B	347	LYS	CA-C	5.51	1.60	1.52
2	B	142	ILE	CA-CB	-5.50	1.47	1.54
1	A	553	SER	CA-C	5.47	1.60	1.52
2	B	132	ILE	CA-C	-5.43	1.47	1.52
1	A	10	VAL	N-CA	-5.42	1.40	1.46
1	A	495	ILE	CA-CB	-5.42	1.47	1.54
2	B	151	GLN	N-CA	-5.42	1.39	1.46
1	A	381	VAL	CA-CB	-5.41	1.48	1.54
2	B	276	VAL	N-CA	5.38	1.53	1.46
1	A	355	ALA	CA-C	-5.34	1.45	1.52
1	A	165	THR	CA-CB	5.31	1.61	1.53
1	A	218	ASP	N-CA	5.31	1.52	1.45
1	A	169	GLU	C-O	-5.31	1.19	1.24
2	B	407	GLN	CG-CD	5.28	1.65	1.52
1	A	319	TYR	C-O	-5.27	1.17	1.23
2	B	37	ILE	C-O	-5.25	1.17	1.24
2	B	26	LEU	C-O	-5.22	1.17	1.23
1	A	377	THR	C-O	-5.13	1.18	1.24
1	A	148	VAL	C-O	-5.11	1.17	1.23
1	A	510	PRO	CA-C	-5.10	1.46	1.52
2	B	76	ASP	N-CA	-5.09	1.40	1.46
1	A	188	TYR	CA-C	-5.08	1.46	1.52
2	B	423	VAL	CA-CB	5.08	1.60	1.54
1	A	33	ALA	CA-CB	-5.07	1.45	1.53
2	B	363	ASN	N-CA	5.07	1.52	1.45
1	A	387	PRO	N-CA	-5.00	1.41	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	PRO	CA-C-N	8.78	136.31	122.61
1	A	345	PRO	C-N-CA	8.78	136.31	122.61
1	A	420	PRO	O-C-N	8.30	125.05	121.15
2	B	348	ASN	N-CA-C	7.39	120.95	110.23
1	A	38	CYS	N-CA-C	6.94	118.84	111.28
1	A	54	ASN	N-CA-C	-6.87	99.26	109.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	VAL	N-CA-C	6.77	117.28	108.35
1	A	545	ASN	N-CA-C	-6.68	103.92	111.07
1	A	409	THR	N-CA-C	-6.41	98.16	109.06
2	B	111	VAL	CB-CA-C	-6.37	103.89	111.65
2	B	13	LYS	N-CA-C	6.28	123.69	109.81
2	B	24	TRP	CA-C-N	6.24	126.26	119.90
2	B	24	TRP	C-N-CA	6.24	126.26	119.90
1	A	346	PHE	CB-CA-C	6.13	121.22	111.48
2	B	276	VAL	CB-CA-C	-6.06	101.34	111.29
2	B	190	GLY	N-CA-C	6.05	121.47	110.71
1	A	79	GLU	N-CA-C	6.03	117.52	111.07
1	A	345	PRO	O-C-N	6.03	130.78	122.64
1	A	346	PHE	N-CA-C	6.02	119.93	112.47
2	B	326	ILE	CB-CA-C	5.94	119.97	110.82
2	B	156	SER	CA-C-N	-5.90	112.94	119.19
2	B	156	SER	C-N-CA	-5.90	112.94	119.19
2	B	118	VAL	CB-CA-C	-5.88	105.47	110.94
1	A	147	ASN	N-CA-C	-5.85	106.12	113.72
2	B	18	GLY	N-CA-C	5.84	119.01	112.00
2	B	270	ILE	CB-CA-C	-5.84	105.85	111.05
1	A	3	SER	CA-C-N	5.83	125.53	119.64
1	A	3	SER	C-N-CA	5.83	125.53	119.64
2	B	13	LYS	CA-C-N	-5.77	112.62	119.84
2	B	13	LYS	C-N-CA	-5.77	112.62	119.84
1	A	463	ARG	N-CA-C	5.72	117.68	110.24
2	B	106	VAL	CB-CA-C	-5.72	102.16	110.63
1	A	161	GLN	N-CA-C	-5.72	104.50	112.45
1	A	182	GLN	N-CA-CB	-5.72	100.94	110.37
2	B	169	GLU	CA-C-N	-5.71	112.70	119.84
2	B	169	GLU	C-N-CA	-5.71	112.70	119.84
2	B	118	VAL	N-CA-C	5.71	113.54	108.63
1	A	553	SER	N-CA-C	5.71	120.24	113.16
1	A	163	SER	N-CA-C	-5.69	104.76	110.97
1	A	513	SER	N-CA-C	5.68	117.71	109.07
2	B	198	HIS	N-CA-C	-5.65	105.02	111.07
1	A	131	THR	CA-C-N	-5.47	118.65	122.59
1	A	131	THR	C-N-CA	-5.47	118.65	122.59
1	A	461	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	A	521	ILE	CB-CA-C	-5.45	104.79	112.14
1	A	388	LYS	N-CA-C	-5.41	100.42	109.24
2	B	381	VAL	CB-CA-C	-5.41	104.95	112.04
1	A	189	VAL	N-CA-C	5.33	116.26	108.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	114	ALA	N-CA-C	5.33	117.50	111.11
1	A	462	GLY	N-CA-C	5.26	121.09	114.25
1	A	117	SER	N-CA-C	5.22	119.36	113.15
1	A	177	ASP	CA-C-N	5.19	127.56	120.35
1	A	177	ASP	C-N-CA	5.19	127.56	120.35
2	B	60	VAL	CB-CA-C	-5.16	102.88	110.82
2	B	420	PRO	CA-C-N	5.12	126.24	119.84
2	B	420	PRO	C-N-CA	5.12	126.24	119.84
1	A	414	TRP	N-CA-C	5.11	116.58	108.96
1	A	225	PRO	N-CA-C	5.11	116.94	110.70
1	A	317	VAL	N-CA-CB	-5.04	106.60	112.34

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	4485	0	4530	138	0
2	B	3320	0	3341	98	0
3	A	28	0	15	3	0
4	A	169	0	0	19	0
4	B	136	0	0	10	0
All	All	8138	0	7886	230	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 15.

All (230) 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:80:LEU:O	1:A:84:THR:HG22	1.39	1.18
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.33	1.09
1:A:409:THR:HG21	4:A:695:HOH:O	1.63	0.98
1:A:428:GLN:NE2	1:A:431:LYS:HZ1	1.61	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HG21	4:A:722:HOH:O	1.64	0.96
1:A:428:GLN:HE22	1:A:431:LYS:HZ1	1.04	0.92
1:A:428:GLN:NE2	1:A:431:LYS:NZ	2.20	0.89
1:A:428:GLN:HE22	1:A:431:LYS:NZ	1.75	0.83
1:A:31:ILE:O	1:A:35:VAL:HG23	1.78	0.83
2:B:326:ILE:HD11	2:B:390:LYS:HG3	1.59	0.83
2:B:283:LEU:HA	2:B:287:LYS:HZ1	1.44	0.83
1:A:406:TRP:HZ3	4:A:708:HOH:O	1.61	0.82
1:A:268:SER:O	1:A:351:THR:HG22	1.81	0.81
2:B:240:THR:HG22	4:B:485:HOH:O	1.84	0.78
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.65	0.77
2:B:214:LEU:O	4:B:557:HOH:O	2.02	0.77
2:B:211:ARG:O	2:B:212:TRP:HB2	1.84	0.76
1:A:51:GLY:CA	1:A:53:GLU:OE1	2.34	0.75
2:B:91:GLN:O	2:B:92:LEU:HD12	1.85	0.75
1:A:37:ILE:CG2	1:A:41:MET:HE2	2.16	0.74
3:A:562:65B:N12	3:A:562:65B:H22	2.00	0.74
2:B:283:LEU:HA	2:B:287:LYS:NZ	2.02	0.74
1:A:80:LEU:O	1:A:84:THR:CG2	2.28	0.73
2:B:296:THR:HG22	2:B:297:GLU:N	2.03	0.73
1:A:215:THR:HG23	4:A:703:HOH:O	1.90	0.72
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.71	0.72
1:A:106:VAL:HG22	1:A:227:PHE:CE2	2.24	0.72
1:A:411:ILE:HD11	1:A:414:TRP:CD1	2.25	0.71
1:A:51:GLY:HA3	1:A:53:GLU:OE1	1.91	0.71
2:B:365:VAL:O	2:B:369:THR:HG23	1.91	0.70
1:A:27:THR:HG22	1:A:30:LYS:HG3	1.74	0.70
2:B:91:GLN:C	2:B:92:LEU:HD12	2.18	0.69
1:A:23:GLN:OE1	1:A:60:VAL:HG23	1.94	0.68
2:B:347:LYS:O	4:B:553:HOH:O	2.11	0.67
2:B:214:LEU:C	4:B:557:HOH:O	2.37	0.67
1:A:178:ILE:CD1	1:A:191:SER:HB3	2.24	0.66
2:B:186:ASP:OD2	4:B:560:HOH:O	2.14	0.66
2:B:191:SER:OG	2:B:198:HIS:ND1	2.24	0.66
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.59	0.66
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.31	0.65
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.78	0.65
1:A:435:VAL:HG13	2:B:290:THR:OG1	1.96	0.65
2:B:314:VAL:HB	2:B:317:VAL:CG2	2.26	0.65
2:B:418:ASN:HB2	4:B:523:HOH:O	1.96	0.64
2:B:296:THR:CG2	2:B:297:GLU:N	2.59	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG22	1:A:227:PHE:CZ	2.31	0.64
1:A:37:ILE:HG22	1:A:41:MET:CE	2.20	0.64
1:A:246:LEU:N	1:A:246:LEU:HD23	2.12	0.64
1:A:325:LEU:C	1:A:326:ILE:HD12	2.22	0.64
1:A:178:ILE:HD12	1:A:191:SER:HB3	1.79	0.63
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.33	0.63
2:B:191:SER:HG	2:B:198:HIS:HD1	1.44	0.62
1:A:428:GLN:HB2	4:A:650:HOH:O	2.01	0.61
2:B:317:VAL:HG12	2:B:347:LYS:HB3	1.82	0.61
2:B:211:ARG:O	2:B:212:TRP:CB	2.46	0.61
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.82	0.61
1:A:300:GLU:HG3	4:A:725:HOH:O	2.00	0.60
1:A:39:THR:HG22	1:A:43:LYS:HD3	1.83	0.60
2:B:312:GLU:HG3	2:B:313:PRO:HD2	1.84	0.60
1:A:27:THR:O	1:A:31:ILE:HG13	2.01	0.60
1:A:32:LYS:NZ	1:A:36:GLU:OE1	2.34	0.60
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.67	0.60
1:A:27:THR:CG2	1:A:30:LYS:HG3	2.32	0.60
1:A:58:THR:HG23	4:A:586:HOH:O	2.01	0.60
1:A:261:VAL:HG13	1:A:276:VAL:HG21	1.84	0.60
1:A:406:TRP:CZ3	4:A:708:HOH:O	2.43	0.59
1:A:461:ARG:NE	4:A:702:HOH:O	2.33	0.59
2:B:84:THR:O	2:B:84:THR:HG22	2.02	0.59
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.84	0.59
1:A:261:VAL:HG13	1:A:276:VAL:CG2	2.33	0.58
2:B:253:THR:HG23	2:B:256:ASP:OD2	2.03	0.58
2:B:276:VAL:HG12	2:B:276:VAL:O	2.03	0.57
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.87	0.57
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.39	0.57
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.85	0.57
1:A:409:THR:CG2	4:A:695:HOH:O	2.38	0.57
2:B:323:LYS:O	2:B:385:LYS:NZ	2.37	0.57
1:A:406:TRP:NE1	4:A:720:HOH:O	2.34	0.57
2:B:296:THR:HG22	2:B:298:GLU:H	1.68	0.57
1:A:169:GLU:N	1:A:170:PRO:HD2	2.20	0.56
2:B:254:VAL:HG13	2:B:283:LEU:HD21	1.87	0.56
2:B:296:THR:HB	2:B:299:ALA:CB	2.36	0.56
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.20	0.55
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.41	0.55
1:A:461:ARG:HH21	1:A:461:ARG:HG3	1.72	0.55
2:B:64:LYS:C	2:B:407:GLN:HE22	2.15	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:VAL:CG1	2:B:347:LYS:HB3	2.36	0.54
1:A:51:GLY:C	1:A:53:GLU:OE1	2.51	0.54
1:A:428:GLN:HG3	1:A:428:GLN:O	2.08	0.54
2:B:12:LEU:O	2:B:14:PRO:CD	2.55	0.54
2:B:314:VAL:HB	2:B:317:VAL:HG21	1.90	0.53
1:A:203:GLU:OE2	1:A:219:LYS:HG2	2.09	0.53
2:B:314:VAL:HB	2:B:317:VAL:HG22	1.90	0.53
2:B:295:LEU:HD13	2:B:300:GLU:OE1	2.09	0.53
1:A:244:ILE:HG22	1:A:246:LEU:HD21	1.91	0.52
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.43	0.52
1:A:466:VAL:HG21	1:A:551:LEU:HD13	1.90	0.52
2:B:12:LEU:O	2:B:14:PRO:HD2	2.09	0.52
2:B:111:VAL:HG22	2:B:185:ASP:O	2.10	0.52
2:B:58:THR:HG23	2:B:76:ASP:O	2.10	0.52
1:A:27:THR:HG22	1:A:30:LYS:CG	2.40	0.51
1:A:485:ALA:O	1:A:489:SER:HB2	2.10	0.51
1:A:98:ALA:HB1	1:A:383:TRP:HZ2	1.75	0.51
1:A:171:PHE:CD1	1:A:171:PHE:C	2.89	0.51
2:B:250:ASP:CG	2:B:251:SER:N	2.68	0.51
2:B:252:TRP:CH2	2:B:260:LEU:HD22	2.45	0.51
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.93	0.51
1:A:178:ILE:HD11	1:A:191:SER:HB3	1.92	0.51
1:A:544:GLY:O	1:A:548:VAL:HG23	2.11	0.51
1:A:64:LYS:NZ	1:A:69:THR:O	2.42	0.51
2:B:101:LYS:O	2:B:236:PRO:HB2	2.11	0.51
1:A:402:TRP:CE2	1:A:403:THR:HG22	2.46	0.51
2:B:43:LYS:HD2	4:B:532:HOH:O	2.11	0.50
1:A:168:LEU:O	1:A:169:GLU:C	2.54	0.50
1:A:286:THR:N	4:A:726:HOH:O	2.45	0.50
1:A:411:ILE:HD11	1:A:414:TRP:CG	2.45	0.50
1:A:93:GLY:HA3	2:B:137:ASN:ND2	2.26	0.50
1:A:168:LEU:C	1:A:170:PRO:HD2	2.37	0.50
1:A:134:SER:OG	1:A:139:THR:O	2.21	0.50
2:B:82:LYS:HD2	2:B:413:GLU:OE2	2.12	0.50
2:B:300:GLU:HG3	4:B:566:HOH:O	2.12	0.50
2:B:254:VAL:HG13	2:B:283:LEU:CD2	2.42	0.49
1:A:466:VAL:CG2	1:A:551:LEU:HD13	2.43	0.49
1:A:503:LEU:HG	1:A:507:GLN:HG3	1.94	0.49
1:A:286:THR:C	1:A:287:LYS:HD2	2.38	0.49
1:A:75:VAL:HG12	1:A:76:ASP:N	2.28	0.49
2:B:274:ILE:HD13	2:B:309:ILE:CD1	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:MET:HE3	4:A:578:HOH:O	2.13	0.49
2:B:246:LEU:HD12	2:B:307:ARG:HG3	1.95	0.49
1:A:210:LEU:C	1:A:212:TRP:H	2.20	0.48
1:A:178:ILE:HD12	1:A:191:SER:CB	2.43	0.48
1:A:443:ASP:O	1:A:481:ALA:HB2	2.14	0.48
2:B:296:THR:HB	2:B:299:ALA:HB3	1.94	0.48
1:A:244:ILE:HG22	1:A:246:LEU:CD2	2.44	0.48
1:A:81:ASN:HA	1:A:84:THR:HG23	1.94	0.48
1:A:460:ASN:HD21	1:A:461:ARG:NH2	2.11	0.48
1:A:406:TRP:CD1	4:A:720:HOH:O	2.66	0.48
2:B:296:THR:HG22	2:B:298:GLU:N	2.28	0.48
1:A:181:TYR:HB2	3:A:562:65B:BR	2.70	0.47
4:A:590:HOH:O	2:B:394:GLN:HG3	2.13	0.47
1:A:169:GLU:N	1:A:170:PRO:CD	2.77	0.47
1:A:211:ARG:HG3	4:A:643:HOH:O	2.14	0.47
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.50	0.47
3:A:562:65B:N12	3:A:562:65B:C22	2.67	0.47
2:B:157:PRO:HG3	2:B:184:MET:HA	1.95	0.47
2:B:326:ILE:HD12	2:B:388:LYS:O	2.14	0.47
2:B:250:ASP:CG	2:B:251:SER:H	2.23	0.47
2:B:276:VAL:O	2:B:276:VAL:CG1	2.62	0.47
1:A:266:TRP:O	1:A:269:GLN:HG3	2.15	0.47
2:B:79:GLU:OE1	2:B:83:ARG:NH1	2.48	0.46
1:A:156:SER:N	1:A:157:PRO:CD	2.79	0.46
1:A:260:LEU:HD22	1:A:264:LEU:HG	1.98	0.46
1:A:461:ARG:CD	4:A:702:HOH:O	2.63	0.46
1:A:257:ILE:O	1:A:261:VAL:HG23	2.15	0.46
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.50	0.46
1:A:210:LEU:C	1:A:212:TRP:N	2.72	0.46
1:A:445:ALA:O	1:A:477:THR:HG21	2.16	0.46
1:A:10:VAL:HG12	1:A:11:LYS:N	2.31	0.45
1:A:10:VAL:HG12	1:A:11:LYS:H	1.81	0.45
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.45	0.45
2:B:286:THR:O	2:B:286:THR:HG22	2.17	0.45
1:A:2:ILE:O	1:A:3:SER:C	2.60	0.45
1:A:287:LYS:HG3	1:A:291:GLU:OE1	2.17	0.45
1:A:69:THR:HG22	1:A:70:LYS:H	1.81	0.45
1:A:402:TRP:CE2	1:A:403:THR:CG2	3.00	0.45
1:A:504:GLY:O	1:A:505:ILE:C	2.60	0.45
1:A:412:PRO:O	1:A:413:GLU:C	2.60	0.44
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:O	2:B:247:PRO:C	2.60	0.44
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.18	0.44
1:A:437:ALA:HB3	1:A:494:ASN:ND2	2.32	0.44
2:B:211:ARG:N	2:B:211:ARG:HD2	2.32	0.44
2:B:292:VAL:CG2	2:B:293:ILE:N	2.80	0.44
1:A:270:ILE:HA	1:A:351:THR:HB	2.00	0.44
1:A:139:THR:HB	1:A:140:PRO:HD2	2.00	0.44
1:A:297:GLU:O	1:A:301:LEU:HD13	2.18	0.44
1:A:500:GLN:OE1	2:B:422:LEU:HD12	2.18	0.44
2:B:303:LEU:HD22	2:B:307:ARG:NH1	2.32	0.44
2:B:283:LEU:HD23	2:B:287:LYS:HZ3	1.83	0.43
1:A:538:ALA:HB1	1:A:539:HIS:CD2	2.53	0.43
1:A:407:GLN:HG3	4:A:708:HOH:O	2.18	0.43
2:B:274:ILE:HD13	2:B:309:ILE:HD13	2.00	0.43
2:B:373:GLN:NE2	4:B:552:HOH:O	2.50	0.43
1:A:211:ARG:HD2	4:A:638:HOH:O	2.18	0.43
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.53	0.43
2:B:10:VAL:HG12	2:B:11:LYS:N	2.33	0.43
2:B:108:VAL:HG22	2:B:188:TYR:CD1	2.53	0.43
2:B:180:ILE:HG21	2:B:180:ILE:HD13	1.75	0.43
2:B:213:GLY:O	2:B:214:LEU:HG	2.18	0.43
2:B:405:TYR:O	2:B:407:GLN:HG2	2.18	0.43
1:A:53:GLU:OE2	1:A:54:ASN:N	2.51	0.43
1:A:328:GLU:HG2	1:A:390:LYS:HB2	2.01	0.43
2:B:336:GLN:C	2:B:337:TRP:CD1	2.97	0.43
1:A:28:GLU:O	1:A:29:GLU:C	2.62	0.43
2:B:106:VAL:HG12	2:B:107:THR:N	2.32	0.43
2:B:278:GLN:O	2:B:281:LYS:HB2	2.18	0.43
2:B:303:LEU:HD22	2:B:307:ARG:HH12	1.84	0.43
2:B:195:ILE:HD12	2:B:195:ILE:HA	1.68	0.42
1:A:17:ASP:O	1:A:83:ARG:NH1	2.43	0.42
1:A:461:ARG:HH21	1:A:461:ARG:CG	2.32	0.42
1:A:446:ALA:HB3	1:A:474:ASN:HD22	1.85	0.42
2:B:191:SER:HB2	2:B:193:LEU:HD22	2.01	0.42
2:B:120:LEU:O	2:B:121:ASP:C	2.63	0.42
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.55	0.42
2:B:5:ILE:HG22	2:B:119:PRO:HD2	2.01	0.42
1:A:103:LYS:O	1:A:236:PRO:HB3	2.19	0.42
1:A:120:LEU:O	1:A:121:ASP:C	2.62	0.42
1:A:437:ALA:HB3	1:A:494:ASN:HD21	1.84	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PHE:O	2:B:125:ARG:C	2.61	0.42
1:A:54:ASN:O	1:A:143:ARG:NH2	2.53	0.42
1:A:479:LEU:HD23	1:A:517:LEU:HD13	2.01	0.42
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.20	0.41
2:B:108:VAL:HG22	2:B:188:TYR:CE1	2.55	0.41
2:B:241:VAL:HG12	2:B:351:THR:H	1.85	0.41
1:A:228:LEU:HD22	1:A:242:GLN:HG2	2.03	0.41
1:A:90:VAL:HG12	1:A:91:GLN:N	2.35	0.41
1:A:498:ASP:HA	1:A:536:VAL:O	2.21	0.41
2:B:306:ASN:O	2:B:307:ARG:C	2.64	0.41
1:A:59:PRO:O	1:A:75:VAL:HG13	2.20	0.41
1:A:277:ARG:HB2	1:A:336:GLN:HE21	1.84	0.41
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.56	0.40
2:B:42:GLU:O	2:B:43:LYS:C	2.62	0.40
1:A:203:GLU:O	1:A:204:GLU:C	2.63	0.40
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.56	0.40
2:B:422:LEU:O	2:B:423:VAL:C	2.64	0.40
1:A:327:ALA:O	1:A:389:PHE:HA	2.22	0.40
1:A:443:ASP:CG	1:A:444:GLY:H	2.29	0.40
2:B:413:GLU:CD	4:B:493:HOH:O	2.64	0.40
2:B:261:VAL:HG13	2:B:276:VAL:HG11	2.03	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	547/561 (98%)	509 (93%)	34 (6%)	4 (1%)	18	37
2	B	393/440 (89%)	364 (93%)	21 (5%)	8 (2%)	6	14
All	All	940/1001 (94%)	873 (93%)	55 (6%)	12 (1%)	9	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
2	B	13	LYS
1	A	471	ASP
2	B	14	PRO
2	B	22	LYS
2	B	277	ARG
2	B	347	LYS
1	A	52	PRO
1	A	413	GLU
2	B	121	ASP
2	B	212	TRP
2	B	133	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	491/501 (98%)	426 (87%)	65 (13%)	4	8
2	B	365/400 (91%)	328 (90%)	37 (10%)	7	16
All	All	856/901 (95%)	754 (88%)	102 (12%)	5	11

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	21	VAL
1	A	27	THR
1	A	29	GLU
1	A	43	LYS
1	A	53	GLU
1	A	60	VAL
1	A	64	LYS
1	A	73	LYS
1	A	74	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	84	THR
1	A	89	GLU
1	A	91	GLN
1	A	106	VAL
1	A	138	GLU
1	A	178	ILE
1	A	179	VAL
1	A	185	ASP
1	A	187	LEU
1	A	194	GLU
1	A	195	ILE
1	A	197	GLN
1	A	201	LYS
1	A	207	GLN
1	A	211	ARG
1	A	215	THR
1	A	216	THR
1	A	219	LYS
1	A	224	GLU
1	A	230	MET
1	A	245	VAL
1	A	249	LYS
1	A	260	LEU
1	A	276	VAL
1	A	280	CYS
1	A	289	LEU
1	A	295	LEU
1	A	298	GLU
1	A	300	GLU
1	A	317	VAL
1	A	325	LEU
1	A	334	GLN
1	A	345	PRO
1	A	347	LYS
1	A	351	THR
1	A	357	MET
1	A	361	HIS
1	A	388	LYS
1	A	411	ILE
1	A	425	LEU
1	A	428	GLN
1	A	435	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	442	VAL
1	A	454	LYS
1	A	461	ARG
1	A	464	GLN
1	A	474	ASN
1	A	507	GLN
1	A	517	LEU
1	A	529	GLU
1	A	540	LYS
1	A	547	GLN
1	A	548	VAL
1	A	552	VAL
2	B	6	GLU
2	B	11	LYS
2	B	12	LEU
2	B	42	GLU
2	B	73	LYS
2	B	74	LEU
2	B	90	VAL
2	B	91	GLN
2	B	139	THR
2	B	179	VAL
2	B	193	LEU
2	B	195	ILE
2	B	202	ILE
2	B	214	LEU
2	B	232	TYR
2	B	245	VAL
2	B	248	GLU
2	B	255	ASN
2	B	257	ILE
2	B	263	LYS
2	B	287	LYS
2	B	290	THR
2	B	292	VAL
2	B	293	ILE
2	B	295	LEU
2	B	301	LEU
2	B	303	LEU
2	B	314	VAL
2	B	317	VAL
2	B	326	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	353	LYS
2	B	385	LYS
2	B	388	LYS
2	B	403	THR
2	B	409	THR
2	B	423	VAL
2	B	424	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	147	ASN
1	A	182	GLN
1	A	198	HIS
1	A	336	GLN
1	A	373	GLN
1	A	428	GLN
1	A	474	ASN
1	A	480	GLN
1	A	509	GLN
1	A	520	GLN
1	A	539	HIS
2	B	147	ASN
2	B	182	GLN
2	B	208	HIS
2	B	278	GLN
2	B	367	GLN
2	B	394	GLN
2	B	407	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	65B	A	562	-	30,30,30	1.49	5 (16%)	40,42,42	2.96	20 (50%)

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	562	-	-	0/12/12/12	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	562	65B	C13-C14	-3.79	1.33	1.38
3	A	562	65B	C15-N16	-2.93	1.31	1.35
3	A	562	65B	C3-C2	-2.84	1.35	1.39
3	A	562	65B	C3-C4	2.09	1.43	1.39
3	A	562	65B	C11-N5	2.07	1.40	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	562	65B	C11-N16-C15	7.17	122.41	116.59
3	A	562	65B	O17-C13-C14	-6.19	113.90	117.89
3	A	562	65B	BR-C14-C13	-4.86	114.74	121.55
3	A	562	65B	C14-C13-N12	-4.82	118.60	123.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	562	65B	O17-C13-N12	4.70	127.49	119.61
3	A	562	65B	C14-C15-N18	-4.55	118.71	122.76
3	A	562	65B	N18-C15-N16	4.50	123.10	117.03
3	A	562	65B	N16-C11-N12	-4.27	119.26	126.26
3	A	562	65B	C4-C5-C6	-3.55	115.97	121.06
3	A	562	65B	C5-C4-C4'	-3.40	114.97	119.55
3	A	562	65B	C6'-C6-C1	-3.15	115.75	120.80
3	A	562	65B	C11-N12-C13	3.12	120.75	115.38
3	A	562	65B	BR-C14-C15	3.08	124.50	120.70
3	A	562	65B	C2'-C2-C1	-3.07	115.88	120.80
3	A	562	65B	C25-C26-C21	-2.63	117.27	120.30
3	A	562	65B	C5-C6-C1	2.54	121.62	117.94
3	A	562	65B	C3-C2-C1	2.49	121.55	117.94
3	A	562	65B	C21-N5-C11	-2.34	123.08	129.38
3	A	562	65B	C4-C3-C2	-2.23	117.85	121.06
3	A	562	65B	C3-C4-C4'	2.05	122.32	119.55

There are no chirality outliers.

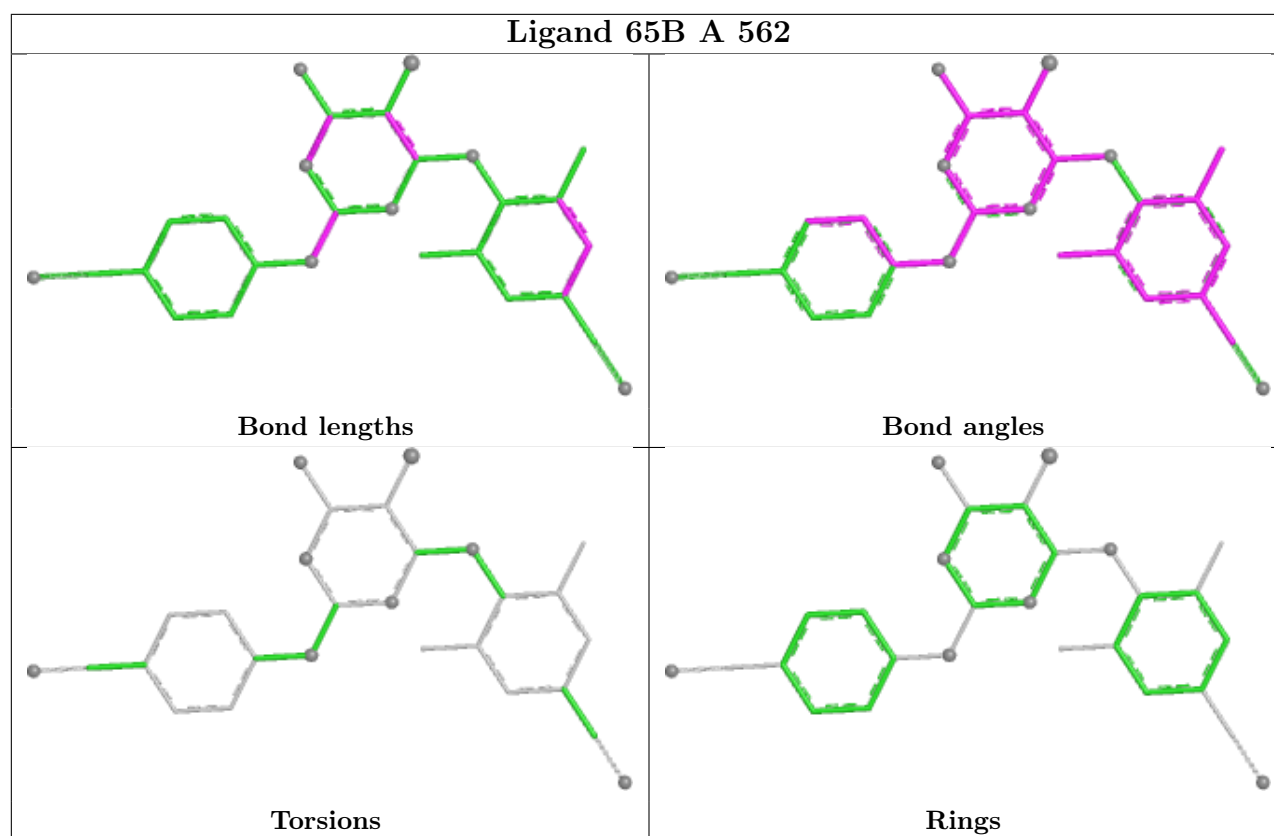
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	562	65B	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	551/561 (98%)	-0.06	9 (1%) 70 68	25, 49, 75, 103	0
2	B	401/440 (91%)	-0.07	10 (2%) 58 54	26, 46, 82, 95	0
All	All	952/1001 (95%)	-0.06	19 (1%) 65 61	25, 48, 79, 103	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	LYS	3.8
1	A	555	GLY	3.1
1	A	222	GLN	3.1
2	B	232	TYR	3.0
2	B	229	TRP	2.8
2	B	13	LYS	2.8
2	B	293	ILE	2.7
2	B	295	LEU	2.6
1	A	286	THR	2.5
1	A	223	LYS	2.5
2	B	5	ILE	2.4
2	B	231	GLY	2.4
1	A	221	HIS	2.3
1	A	91	GLN	2.2
1	A	409	THR	2.1
1	A	554	ALA	2.1
2	B	24	TRP	2.1
2	B	16	MET	2.1
2	B	292	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

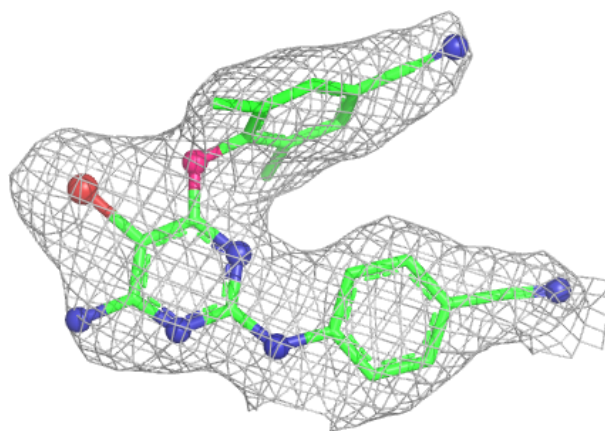
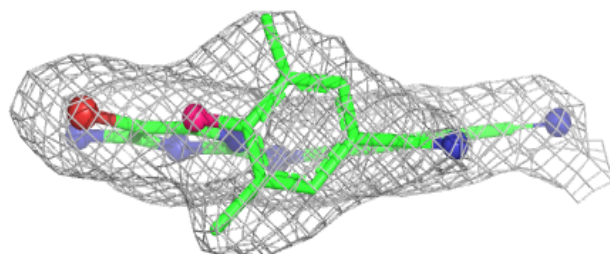
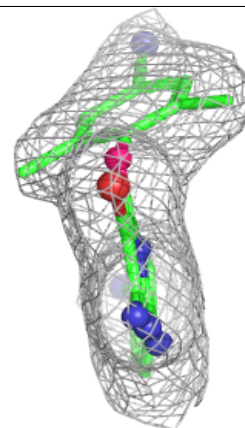
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	65B	A	562	28/28	0.97	0.06	24,33,40,45	1

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 562:

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.