



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:03 AM UTC

PDB ID : 1TKX / pdb_00001tkx
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN
COMPLEX WITH GW490745
Authors : Ren, J.; Hopkins, A.L.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2004-06-09
Resolution : 2.85 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

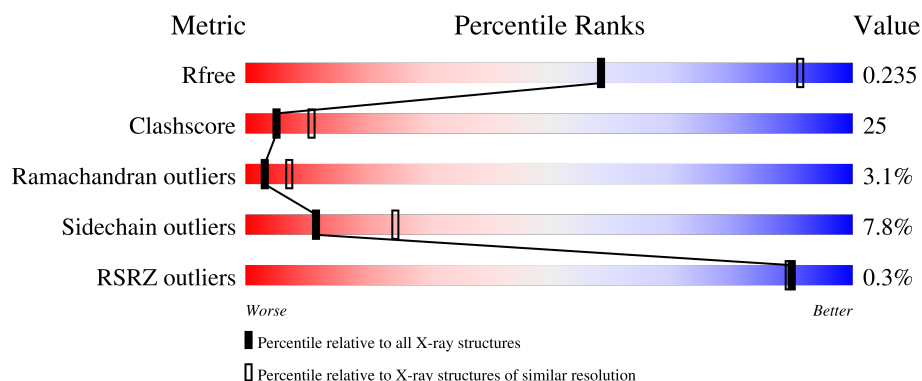
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

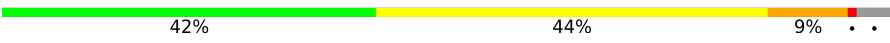
The reported resolution of this entry is 2.85 Å.

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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 7745 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 Pol polyprotein, Reverse transcriptase, Chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4381	2835	730	808	8			

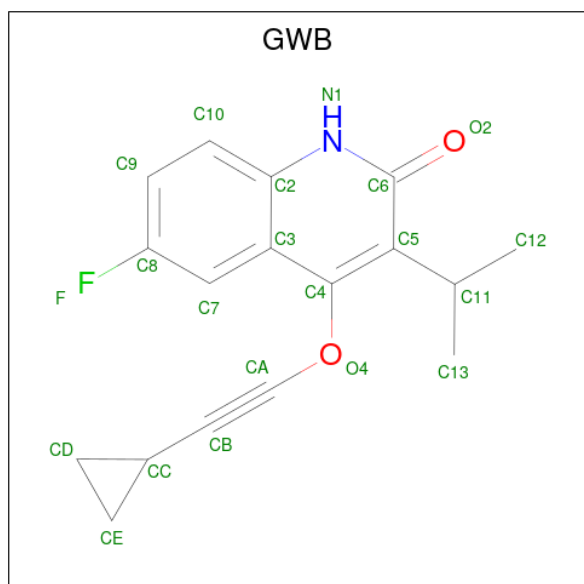
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	modified residue	UNP P04585

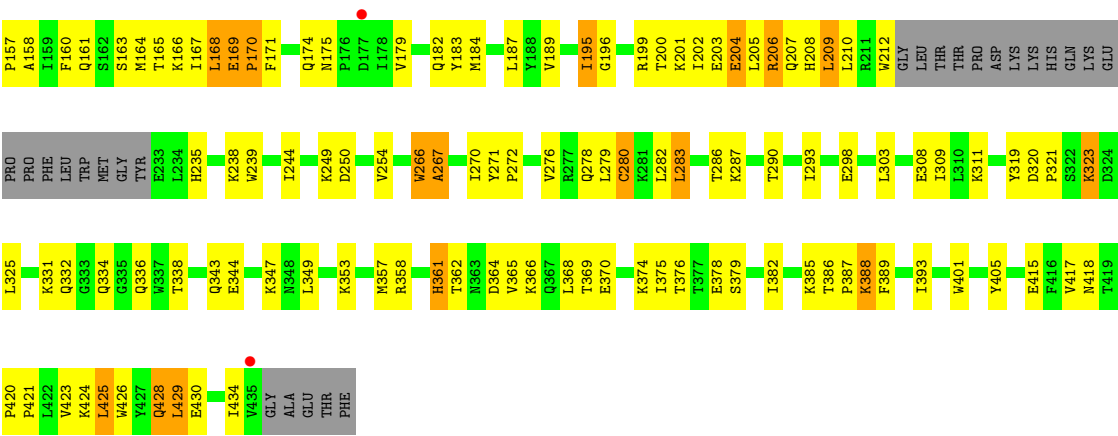
- Molecule 2 is a protein called Pol polyprotein, Reverse transcriptase, Chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3343	2174	555	607	7			

- Molecule 3 is 4-[(CYCLOPROPYLETHYNYL)OXY]-6-FLUORO-3-ISOPROPYLQUINOLIN-2(1H)-ONE (CCD ID: GWB) (formula: C₁₇H₁₆FNO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			21	17	1	1	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.20Å 109.70Å 72.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.85 29.63 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.63-2.85) 98.3 (29.63-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.287 0.211 , 0.235	Depositor DCC
R_{free} test set	1260 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 82.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7745	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: CSD, GWB

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	0.47	0/4488	1.03	24/6099 (0.4%)
2	B	0.47	0/3436	1.02	18/4667 (0.4%)
All	All	0.47	0/7924	1.03	42/10766 (0.4%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	LYS	N-CA-C	-8.86	95.07	109.96
2	B	70	LYS	N-CA-C	-8.54	98.46	110.50
1	A	92	LEU	N-CA-C	-8.37	103.20	113.50
2	B	168	LEU	N-CA-C	8.12	119.90	111.14
2	B	94	ILE	N-CA-C	8.03	116.64	107.89
1	A	245	VAL	N-CA-C	7.09	118.08	107.80
1	A	215	THR	N-CA-C	7.08	119.85	111.71
1	A	54	ASN	N-CA-C	6.99	121.28	108.69
2	B	428	GLN	N-CA-C	-6.59	104.13	111.71
1	A	518	VAL	N-CA-C	-6.46	104.03	110.62
2	B	417	VAL	N-CA-C	6.43	116.37	108.53
1	A	509	GLN	CA-C-N	6.33	126.28	119.76
1	A	509	GLN	C-N-CA	6.33	126.28	119.76
2	B	382	ILE	N-CA-C	6.31	117.32	111.45
2	B	250	ASP	N-CA-C	-6.25	104.39	111.14
2	B	131	THR	N-CA-C	6.19	119.22	108.76
2	B	434	ILE	N-CA-C	-6.13	104.36	110.30
2	B	349	LEU	N-CA-C	-6.05	106.03	113.41
1	A	118	VAL	CA-C-N	5.89	125.83	119.76
1	A	118	VAL	C-N-CA	5.89	125.83	119.76
2	B	115	TYR	N-CA-C	5.86	117.75	111.36
2	B	206	ARG	N-CA-C	-5.74	104.71	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	THR	N-CA-C	5.72	118.82	108.69
2	B	200	THR	N-CA-C	-5.58	104.83	111.69
1	A	233	GLU	N-CA-C	-5.48	99.58	108.52
1	A	241	VAL	N-CA-C	5.48	116.65	108.54
2	B	204	GLU	N-CA-C	-5.46	105.32	111.28
1	A	349	LEU	N-CA-C	-5.40	104.94	112.45
2	B	203	GLU	N-CA-C	-5.40	105.50	111.71
1	A	481	ALA	N-CA-C	-5.35	105.13	110.97
1	A	104	LYS	N-CA-C	-5.35	105.36	111.14
1	A	417	VAL	N-CA-C	-5.30	100.44	108.17
1	A	397	THR	N-CA-C	-5.17	105.53	111.07
1	A	368	LEU	N-CA-C	-5.14	105.57	111.07
1	A	118	VAL	N-CA-C	5.13	113.48	107.89
2	B	266	TRP	N-CA-C	-5.13	105.38	110.97
2	B	147	ASN	N-CA-C	-5.11	107.43	113.97
1	A	527	LYS	N-CA-C	5.08	118.62	112.23
1	A	297	GLU	N-CA-C	-5.07	105.64	111.07
1	A	254	VAL	N-CA-C	-5.04	105.42	110.30
2	B	401	TRP	N-CA-C	5.03	121.83	113.89
1	A	488	ASP	N-CA-C	5.00	119.36	113.16

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	4381	0	4423	253	0
2	B	3343	0	3368	143	0
3	A	21	0	16	3	0
All	All	7745	0	7807	386	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (386) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.45	0.96
1:A:64:LYS:HD3	1:A:64:LYS:O	1.64	0.96
1:A:448:ARG:HE	1:A:474:ASN:H	1.01	0.92
1:A:516:GLU:O	1:A:520:GLN:HG3	1.73	0.89
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.40	0.87
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.37	0.87
1:A:101:LYS:HE3	1:A:101:LYS:N	1.91	0.86
1:A:344:GLU:HG3	1:A:347:LYS:HD2	1.55	0.86
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.61	0.83
1:A:11:LYS:O	1:A:85:GLN:HB3	1.78	0.83
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.61	0.82
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.62	0.82
2:B:163:SER:O	2:B:167:ILE:HG23	1.80	0.82
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.62	0.81
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.62	0.80
1:A:240:THR:HG22	1:A:315:HIS:HB3	1.63	0.80
2:B:175:ASN:ND2	2:B:201:LYS:HD2	1.97	0.79
1:A:31:ILE:O	1:A:35:VAL:HG23	1.83	0.79
1:A:34:LEU:CD2	1:A:73:LYS:HB2	2.13	0.78
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.19	0.78
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.65	0.77
2:B:122:GLU:CG	2:B:125:ARG:NH1	2.48	0.76
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.67	0.76
2:B:31:ILE:O	2:B:35:VAL:HG23	1.86	0.76
2:B:366:LYS:O	2:B:370:GLU:HG3	1.86	0.75
1:A:516:GLU:O	1:A:519:ASN:HB2	1.86	0.75
2:B:170:PRO:O	2:B:174:GLN:HG3	1.87	0.74
2:B:122:GLU:HG2	2:B:125:ARG:NH1	2.04	0.73
1:A:448:ARG:HH21	1:A:475:GLN:H	1.33	0.73
1:A:448:ARG:HE	1:A:474:ASN:N	1.83	0.73
1:A:264:LEU:HD13	1:A:276:VAL:HG12	1.71	0.72
1:A:448:ARG:NE	1:A:474:ASN:H	1.84	0.72
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.72	0.70
1:A:116:PHE:HE1	1:A:146:TYR:HE1	1.39	0.69
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.74	0.69
1:A:170:PRO:O	1:A:174:GLN:HG3	1.93	0.69
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.27	0.69
2:B:27:THR:OG1	2:B:30:LYS:HG3	1.93	0.69
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.57	0.69
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.74	0.68
2:B:122:GLU:HG3	2:B:125:ARG:NH1	2.08	0.68
1:A:122:GLU:H	1:A:122:GLU:CD	2.00	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HA	1:A:226:PRO:C	2.17	0.68
1:A:366:LYS:O	1:A:369:THR:HB	1.93	0.67
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.29	0.67
2:B:235:HIS:O	2:B:238:LYS:HG2	1.95	0.67
2:B:426:TRP:O	2:B:429:LEU:HB2	1.94	0.67
1:A:64:LYS:HD3	1:A:64:LYS:C	2.20	0.67
1:A:344:GLU:CG	1:A:347:LYS:HD2	2.25	0.67
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.10	0.67
1:A:238:LYS:HB2	1:A:316:GLY:O	1.94	0.66
1:A:65:LYS:HB2	1:A:72:ARG:HD2	1.77	0.66
1:A:65:LYS:HG2	1:A:66:LYS:H	1.59	0.66
2:B:338:THR:HG22	2:B:353:LYS:HG3	1.78	0.66
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.31	0.66
1:A:268:SER:HB3	1:A:353:LYS:HE2	1.77	0.65
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.78	0.65
1:A:164:MET:O	1:A:168:LEU:HG	1.97	0.65
1:A:3:SER:OG	1:A:5:ILE:HG13	1.97	0.64
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.29	0.64
1:A:218:ASP:HA	1:A:222:GLN:HG2	1.79	0.64
1:A:116:PHE:CE1	1:A:146:TYR:HE1	2.16	0.63
1:A:475:GLN:HG3	1:A:476:LYS:N	2.14	0.63
1:A:335:GLY:O	1:A:356:ARG:HA	1.99	0.62
1:A:135:ILE:O	1:A:138:GLU:HG3	1.99	0.62
1:A:18:GLY:HA3	1:A:127:TYR:HD1	1.64	0.62
1:A:344:GLU:HG2	1:A:347:LYS:HB2	1.82	0.62
1:A:73:LYS:HE3	1:A:75:VAL:CG2	2.28	0.62
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.82	0.61
2:B:171:PHE:CD2	2:B:205:LEU:HD13	2.35	0.61
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.34	0.61
1:A:253:THR:O	1:A:257:ILE:HG13	2.00	0.61
2:B:122:GLU:CG	2:B:125:ARG:HH12	2.14	0.61
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.35	0.61
1:A:475:GLN:HG3	1:A:476:LYS:H	1.65	0.61
1:A:317:VAL:HG12	1:A:318:TYR:N	2.16	0.61
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.24	0.60
1:A:34:LEU:HD23	1:A:73:LYS:HB2	1.83	0.60
1:A:244:ILE:CG2	1:A:310:LEU:HD13	2.30	0.60
2:B:53:GLU:CD	2:B:53:GLU:H	2.09	0.60
1:A:257:ILE:O	1:A:261:VAL:HG23	2.01	0.60
1:A:170:PRO:HG2	1:A:171:PHE:H	1.67	0.60
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLN:CB	1:A:351:THR:HG22	2.32	0.59
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.37	0.59
2:B:111:VAL:CG1	2:B:187:LEU:HD22	2.30	0.59
2:B:379:SER:OG	2:B:387:PRO:HD3	2.02	0.59
1:A:240:THR:HG22	1:A:315:HIS:CB	2.32	0.59
2:B:84:THR:HB	2:B:154:LYS:HE2	1.84	0.59
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.02	0.59
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.68	0.59
2:B:125:ARG:NE	2:B:147:ASN:HA	2.18	0.59
2:B:365:VAL:O	2:B:369:THR:HG23	2.03	0.59
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.83	0.58
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.84	0.58
1:A:312:GLU:HG2	1:A:313:PRO:HD2	1.84	0.58
1:A:360:ALA:HA	1:A:514:GLU:HB3	1.86	0.57
1:A:65:LYS:CB	1:A:72:ARG:HD2	2.35	0.57
2:B:308:GLU:O	2:B:311:LYS:HB2	2.03	0.57
1:A:18:GLY:HA3	1:A:127:TYR:CD1	2.40	0.57
1:A:194:GLU:O	1:A:197:GLN:N	2.38	0.57
1:A:218:ASP:O	1:A:219:LYS:CB	2.53	0.57
2:B:125:ARG:HE	2:B:147:ASN:HA	1.70	0.56
1:A:402:TRP:CD1	1:A:402:TRP:C	2.83	0.56
1:A:58:THR:HG23	1:A:76:ASP:O	2.05	0.56
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.05	0.56
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.88	0.56
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.41	0.56
1:A:501:TYR:HD2	1:A:501:TYR:O	1.87	0.56
2:B:376:THR:CG2	2:B:386:THR:HG22	2.35	0.56
1:A:420:PRO:HA	1:A:421:PRO:C	2.29	0.56
1:A:100:LEU:C	1:A:101:LYS:HE3	2.31	0.56
1:A:301:LEU:O	1:A:304:ALA:HB3	2.05	0.56
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.41	0.56
2:B:46:LYS:HE2	2:B:116:PHE:CD1	2.41	0.55
1:A:246:LEU:O	1:A:307:ARG:NH1	2.35	0.55
1:A:5:ILE:HD13	1:A:167:ILE:HD11	1.89	0.55
2:B:165:THR:HG23	2:B:166:LYS:H	1.72	0.55
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.42	0.55
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.40	0.55
1:A:92:LEU:HD23	1:A:92:LEU:O	2.05	0.55
1:A:215:THR:O	1:A:216:THR:C	2.48	0.55
1:A:475:GLN:HA	1:A:478:GLU:OE2	2.07	0.55
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HG2	1:A:66:LYS:N	2.22	0.54
1:A:112:GLY:O	1:A:114:ALA:N	2.38	0.54
1:A:90:VAL:O	1:A:91:GLN:C	2.50	0.54
1:A:241:VAL:HG21	1:A:270:ILE:HD13	1.88	0.54
2:B:139:THR:HG22	2:B:140:PRO:O	2.07	0.54
1:A:206:ARG:HH21	1:A:217:PRO:HA	1.70	0.54
2:B:167:ILE:O	2:B:208:HIS:CE1	2.60	0.54
1:A:492:GLU:HA	1:A:530:LYS:O	2.07	0.54
2:B:320:ASP:OD2	2:B:323:LYS:HD3	2.07	0.54
1:A:181:TYR:HB3	1:A:188:TYR:HB2	1.90	0.54
2:B:195:ILE:HG23	2:B:196:GLY:N	2.21	0.54
2:B:154:LYS:O	2:B:157:PRO:HD2	2.08	0.54
1:A:498:ASP:HA	1:A:536:VAL:O	2.07	0.54
2:B:160:PHE:O	2:B:160:PHE:CD1	2.61	0.54
1:A:108:VAL:HG13	1:A:108:VAL:O	2.08	0.54
1:A:173:LYS:O	1:A:176:PRO:HD3	2.09	0.53
2:B:165:THR:HG23	2:B:166:LYS:N	2.22	0.53
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.08	0.53
2:B:23:GLN:HG2	2:B:133:PRO:HD3	1.89	0.53
1:A:253:THR:HA	1:A:291:GLU:O	2.08	0.53
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.44	0.53
1:A:139:THR:HB	1:A:140:PRO:HD2	1.91	0.53
1:A:237:ASP:OD2	1:A:237:ASP:N	2.42	0.53
2:B:344:GLU:HB3	2:B:347:LYS:HE3	1.89	0.53
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.44	0.53
2:B:39:THR:O	2:B:43:LYS:HG2	2.08	0.53
2:B:424:LYS:HD2	2:B:425:LEU:HD13	1.90	0.52
1:A:376:THR:O	1:A:380:ILE:HG12	2.09	0.52
1:A:169:GLU:N	1:A:170:PRO:HD2	2.25	0.52
1:A:34:LEU:HD21	1:A:73:LYS:HB2	1.91	0.52
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.39	0.52
2:B:113:ASP:O	2:B:116:PHE:HD2	1.92	0.52
2:B:19:PRO:O	2:B:20:LYS:HG2	2.09	0.52
2:B:33:ALA:O	2:B:37:ILE:HG13	2.09	0.52
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.43	0.52
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.40	0.52
1:A:134:SER:OG	1:A:138:GLU:HB2	2.10	0.52
1:A:448:ARG:CZ	1:A:473:THR:HB	2.40	0.52
1:A:115:TYR:HD1	1:A:115:TYR:H	1.55	0.52
1:A:225:PRO:HA	1:A:226:PRO:O	2.10	0.52
2:B:11:LYS:N	2:B:85:GLN:OE1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:O	1:A:197:GLN:HB2	2.11	0.51
1:A:293:ILE:N	1:A:293:ILE:HD12	2.25	0.51
2:B:210:LEU:C	2:B:212:TRP:H	2.19	0.51
1:A:163:SER:O	1:A:167:ILE:HG13	2.10	0.51
1:A:206:ARG:HG2	1:A:206:ARG:NH1	2.25	0.51
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.91	0.51
1:A:378:GLU:O	1:A:382:ILE:HG12	2.11	0.51
1:A:518:VAL:O	1:A:522:ILE:HG13	2.11	0.51
1:A:235:HIS:HB2	1:A:238:LYS:O	2.11	0.51
2:B:122:GLU:HG3	2:B:125:ARG:HH12	1.73	0.51
1:A:81:ASN:C	1:A:83:ARG:H	2.19	0.50
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.42	0.50
1:A:64:LYS:HE2	1:A:69:THR:HG23	1.93	0.50
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.91	0.50
2:B:276:VAL:O	2:B:280:CYS:HB2	2.11	0.50
1:A:33:ALA:HB1	1:A:71:TRP:HB3	1.94	0.50
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.12	0.50
1:A:129:ALA:HB1	1:A:143:ARG:NH1	2.26	0.50
1:A:85:GLN:O	1:A:154:LYS:NZ	2.42	0.50
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.38	0.50
1:A:474:ASN:O	1:A:478:GLU:HG3	2.11	0.50
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.47	0.50
1:A:229:TRP:CD2	3:A:999:GWB:HE1	2.47	0.49
1:A:360:ALA:O	1:A:361:HIS:HB3	2.12	0.49
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.12	0.49
2:B:78:ARG:O	2:B:82:LYS:HG3	2.11	0.49
2:B:161:GLN:O	2:B:165:THR:HG22	2.12	0.49
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.47	0.49
2:B:421:PRO:O	2:B:425:LEU:HD22	2.12	0.49
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.46	0.49
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.48	0.49
2:B:379:SER:CB	2:B:387:PRO:HD3	2.42	0.49
1:A:229:TRP:CD1	1:A:230:MET:HG2	2.47	0.48
1:A:460:ASN:HA	2:B:286:THR:O	2.12	0.48
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.95	0.48
1:A:442:VAL:HG22	1:A:496:VAL:O	2.13	0.48
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.48
2:B:287:LYS:HE2	2:B:293:ILE:HD11	1.94	0.48
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.64	0.48
1:A:501:TYR:O	1:A:501:TYR:CD2	2.65	0.48
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.01	0.48
1:A:24:TRP:CG	1:A:61:PHE:HE1	2.31	0.48
1:A:46:LYS:HE2	1:A:116:PHE:CB	2.42	0.48
1:A:69:THR:O	1:A:69:THR:HG22	2.13	0.48
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.95	0.48
2:B:332:GLN:HE22	2:B:424:LYS:HD3	1.78	0.48
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.94	0.48
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.96	0.48
2:B:388:LYS:HE2	2:B:415:GLU:HB3	1.95	0.48
1:A:77:PHE:O	1:A:78:ARG:C	2.56	0.48
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.48	0.48
1:A:98:ALA:HB2	1:A:349:LEU:O	2.14	0.47
1:A:101:LYS:NZ	2:B:138:GLU:OE1	2.46	0.47
1:A:215:THR:O	1:A:216:THR:O	2.32	0.47
1:A:447:ASN:O	1:A:451:LYS:N	2.48	0.47
2:B:202:ILE:O	2:B:205:LEU:HB3	2.14	0.47
1:A:17:ASP:O	1:A:83:ARG:HD3	2.13	0.47
1:A:180:ILE:HG22	1:A:181:TYR:N	2.28	0.47
2:B:331:LYS:NZ	2:B:364:ASP:OD1	2.44	0.47
1:A:122:GLU:OE1	1:A:122:GLU:N	2.42	0.47
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.28	0.47
1:A:139:THR:HB	1:A:140:PRO:CD	2.43	0.47
2:B:167:ILE:HD12	2:B:209:LEU:HD12	1.97	0.47
1:A:57:ASN:HA	1:A:129:ALA:O	2.14	0.47
2:B:118:VAL:HG13	2:B:119:PRO:HD2	1.97	0.47
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.96	0.47
1:A:519:ASN:O	1:A:522:ILE:HB	2.14	0.47
2:B:206:ARG:O	2:B:207:GLN:C	2.58	0.47
1:A:254:VAL:O	1:A:255:ASN:C	2.57	0.47
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.50	0.47
1:A:20:LYS:HZ2	1:A:55:PRO:HB2	1.80	0.46
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.97	0.46
1:A:247:PRO:C	1:A:307:ARG:HH22	2.23	0.46
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.97	0.46
2:B:279:LEU:HA	2:B:282:LEU:HD12	1.98	0.46
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.30	0.46
1:A:184:MET:HB3	1:A:185:ASP:H	1.58	0.46
1:A:477:THR:O	1:A:478:GLU:C	2.57	0.46
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.97	0.46
1:A:176:PRO:C	1:A:178:ILE:H	2.23	0.46
2:B:52:PRO:HD2	2:B:53:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:NE2	2:B:428:GLN:HB2	2.31	0.46
1:A:241:VAL:HB	1:A:314:VAL:HG23	1.96	0.46
2:B:120:LEU:O	2:B:121:ASP:C	2.58	0.46
1:A:104:LYS:HD3	1:A:192:ASP:O	2.16	0.46
2:B:209:LEU:HD12	2:B:209:LEU:HA	1.84	0.45
1:A:58:THR:CG2	1:A:76:ASP:O	2.64	0.45
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.97	0.45
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.30	0.45
1:A:241:VAL:HB	1:A:314:VAL:CG2	2.46	0.45
1:A:281:LYS:O	1:A:284:ARG:HG3	2.16	0.45
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.47	0.45
1:A:125:ARG:NE	1:A:147:ASN:HA	2.32	0.45
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.52	0.45
1:A:206:ARG:NH2	1:A:216:THR:O	2.50	0.45
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.46	0.45
2:B:94:ILE:HD11	2:B:182:GLN:H	1.80	0.45
1:A:218:ASP:HA	1:A:222:GLN:CG	2.46	0.45
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.52	0.45
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.52	0.45
2:B:46:LYS:HE2	2:B:116:PHE:HD1	1.81	0.45
2:B:64:LYS:NZ	2:B:69:THR:O	2.48	0.45
1:A:43:LYS:HD3	1:A:43:LYS:HA	1.60	0.45
1:A:219:LYS:H	1:A:222:GLN:HG3	1.82	0.45
1:A:73:LYS:HG3	1:A:74:LEU:N	2.32	0.44
1:A:402:TRP:CZ2	2:B:362:THR:HA	2.52	0.44
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.52	0.44
2:B:168:LEU:O	2:B:169:GLU:C	2.60	0.44
1:A:96:HIS:O	1:A:97:PRO:C	2.60	0.44
1:A:344:GLU:HG2	1:A:344:GLU:O	2.17	0.44
1:A:408:ALA:HB3	2:B:393:ILE:CG1	2.47	0.44
1:A:501:TYR:CD2	1:A:501:TYR:C	2.96	0.44
1:A:502:ALA:O	1:A:506:ILE:HG13	2.17	0.44
2:B:17:ASP:OD1	2:B:18:GLY:N	2.51	0.44
1:A:27:THR:O	1:A:31:ILE:HG13	2.17	0.44
1:A:81:ASN:C	1:A:83:ARG:N	2.75	0.44
2:B:98:ALA:O	2:B:101:LYS:HE2	2.17	0.44
2:B:118:VAL:CG1	2:B:119:PRO:HD2	2.47	0.44
2:B:357:MET:O	2:B:358:ARG:C	2.60	0.44
1:A:402:TRP:CH2	2:B:362:THR:HA	2.52	0.44
2:B:244:ILE:HG21	2:B:426:TRP:CZ2	2.52	0.44
1:A:183:TYR:CD1	1:A:184:MET:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ILE:O	1:A:384:GLY:HA2	2.18	0.44
1:A:448:ARG:NH2	1:A:475:GLN:H	2.08	0.44
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.99	0.44
2:B:115:TYR:C	2:B:117:SER:N	2.75	0.44
2:B:270:ILE:O	2:B:272:PRO:HD3	2.18	0.44
1:A:279:LEU:HD12	1:A:302:GLU:OE1	2.17	0.43
2:B:325:LEU:HD22	2:B:385:LYS:HD3	1.99	0.43
1:A:9:PRO:HG2	2:B:53:GLU:HG3	1.99	0.43
1:A:241:VAL:CG2	1:A:270:ILE:HD13	2.48	0.43
1:A:71:TRP:HA	1:A:71:TRP:CE3	2.54	0.43
1:A:170:PRO:O	1:A:171:PHE:C	2.61	0.43
1:A:205:LEU:O	1:A:208:HIS:HB3	2.19	0.43
1:A:314:VAL:HG23	1:A:314:VAL:O	2.19	0.43
1:A:317:VAL:CG2	1:A:347:LYS:HB3	2.45	0.43
1:A:340:GLN:HB2	1:A:351:THR:HG22	2.01	0.43
1:A:484:LEU:HD23	1:A:487:GLN:OE1	2.18	0.43
1:A:21:VAL:HG13	1:A:59:PRO:HD3	2.00	0.43
1:A:332:GLN:O	1:A:332:GLN:HG2	2.17	0.43
1:A:84:THR:HB	1:A:154:LYS:HD3	2.01	0.43
2:B:254:VAL:HG21	2:B:287:LYS:HG3	2.01	0.43
1:A:181:TYR:CD1	3:A:999:GWB:HC	2.54	0.43
2:B:195:ILE:HG23	2:B:196:GLY:H	1.82	0.43
1:A:168:LEU:O	1:A:172:ARG:HG3	2.18	0.43
2:B:27:THR:OG1	2:B:30:LYS:CG	2.63	0.43
2:B:51:GLY:HA3	2:B:53:GLU:OE2	2.19	0.43
2:B:344:GLU:CB	2:B:347:LYS:HE3	2.48	0.43
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.19	0.43
2:B:79:GLU:O	2:B:83:ARG:HG3	2.18	0.43
2:B:106:VAL:HA	2:B:189:VAL:O	2.18	0.43
2:B:323:LYS:HB3	2:B:343:GLN:NE2	2.34	0.43
1:A:125:ARG:HB3	1:A:145:GLN:NE2	2.33	0.43
1:A:213:GLY:O	1:A:214:LEU:HD23	2.19	0.42
1:A:448:ARG:HD3	1:A:448:ARG:HA	1.86	0.42
1:A:43:LYS:C	1:A:45:GLY:N	2.74	0.42
2:B:244:ILE:HD13	2:B:430:GLU:HG3	2.01	0.42
1:A:37:ILE:O	1:A:40:GLU:HB3	2.19	0.42
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.54	0.42
1:A:206:ARG:CZ	1:A:216:THR:O	2.68	0.42
1:A:493:VAL:HG12	1:A:494:ASN:N	2.34	0.42
2:B:156:SER:O	2:B:157:PRO:C	2.60	0.42
1:A:65:LYS:O	1:A:69:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.73	0.42
1:A:91:GLN:HE22	1:A:181:TYR:HE2	1.67	0.42
1:A:346:PHE:CD2	1:A:346:PHE:N	2.85	0.42
1:A:363:ASN:HA	1:A:511:ASP:CG	2.45	0.42
2:B:271:TYR:HB3	2:B:309:ILE:HG21	2.00	0.42
2:B:283:LEU:HD12	2:B:283:LEU:HA	1.81	0.42
2:B:334:GLN:O	2:B:336:GLN:OE1	2.37	0.42
2:B:332:GLN:HE22	2:B:428:GLN:HB2	1.84	0.42
1:A:416:PHE:CD1	1:A:417:VAL:N	2.88	0.42
2:B:361:HIS:CD2	2:B:361:HIS:C	2.97	0.42
1:A:79:GLU:O	1:A:80:LEU:C	2.62	0.42
1:A:418:ASN:OD1	1:A:420:PRO:HD3	2.20	0.42
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.81	0.42
1:A:138:GLU:HB3	1:A:139:THR:H	1.66	0.42
1:A:118:VAL:HB	1:A:149:LEU:HD22	2.01	0.41
2:B:239:TRP:CH2	2:B:378:GLU:HA	2.55	0.41
1:A:63:ILE:C	1:A:63:ILE:HD12	2.45	0.41
1:A:216:THR:O	1:A:216:THR:HG23	2.20	0.41
1:A:334:GLN:O	1:A:356:ARG:HD2	2.19	0.41
1:A:336:GLN:HG3	1:A:356:ARG:HB2	2.02	0.41
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.39	0.41
1:A:386:THR:HA	1:A:387:PRO:HD3	1.92	0.41
1:A:491:LEU:O	1:A:529:GLU:N	2.46	0.41
2:B:94:ILE:CD1	2:B:182:GLN:H	2.33	0.41
1:A:426:TRP:HB3	1:A:526:ILE:HG12	2.03	0.41
2:B:139:THR:HG23	2:B:140:PRO:HD2	2.01	0.41
1:A:64:LYS:O	1:A:64:LYS:CD	2.52	0.41
1:A:88:TRP:O	1:A:89:GLU:O	2.37	0.41
1:A:229:TRP:O	1:A:230:MET:C	2.62	0.41
2:B:320:ASP:CG	2:B:323:LYS:HD3	2.46	0.41
1:A:302:GLU:O	1:A:303:LEU:C	2.64	0.41
1:A:270:ILE:HG21	1:A:314:VAL:HG21	2.03	0.41
1:A:317:VAL:CG1	1:A:318:TYR:N	2.82	0.41
1:A:356:ARG:HG2	1:A:358:ARG:NH1	2.36	0.41
2:B:202:ILE:O	2:B:205:LEU:N	2.53	0.41
2:B:134:SER:CB	2:B:139:THR:HB	2.51	0.41
2:B:161:GLN:NE2	2:B:161:GLN:CA	2.76	0.41
1:A:135:ILE:HD12	1:A:135:ILE:N	2.36	0.41
1:A:183:TYR:CD1	1:A:183:TYR:C	2.97	0.41
1:A:255:ASN:HD22	1:A:255:ASN:HA	1.53	0.41
1:A:320:ASP:OD1	1:A:323:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:OD1	1:A:365:VAL:N	2.54	0.41
1:A:410:TRP:CG	1:A:411:ILE:N	2.89	0.41
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.51	0.41
2:B:164:MET:O	2:B:167:ILE:HG12	2.21	0.41
1:A:252:TRP:NE1	1:A:295:LEU:HD11	2.36	0.41
2:B:332:GLN:OE1	2:B:424:LYS:HG2	2.21	0.41
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.56	0.40
1:A:181:TYR:CE1	3:A:999:GWB:HC	2.55	0.40
2:B:98:ALA:O	2:B:101:LYS:HG3	2.21	0.40
2:B:374:LYS:O	2:B:375:ILE:C	2.63	0.40
1:A:493:VAL:HG12	1:A:494:ASN:H	1.86	0.40
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.56	0.40
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.83	0.40
1:A:448:ARG:NE	1:A:473:THR:HB	2.37	0.40
2:B:158:ALA:O	2:B:161:GLN:HB2	2.21	0.40
2:B:201:LYS:O	2:B:204:GLU:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/560 (95%)	462 (87%)	44 (8%)	24 (4%)	2	3
2	B	396/440 (90%)	356 (90%)	35 (9%)	5 (1%)	9	21
All	All	926/1000 (93%)	818 (88%)	79 (8%)	29 (3%)	3	7

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	112	GLY

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Mol	Chain	Res	Type
1	A	216	THR
1	A	91	GLN
1	A	219	LYS
1	A	356	ARG
1	A	361	HIS
2	B	195	ILE
1	A	114	ALA
1	A	170	PRO
1	A	195	ILE
1	A	4	PRO
1	A	14	PRO
1	A	138	GLU
1	A	177	ASP
2	B	267	ALA
1	A	52	PRO
1	A	97	PRO
1	A	111	VAL
1	A	116	PHE
2	B	361	HIS
1	A	82	LYS
1	A	85	GLN
1	A	113	ASP
1	A	412	PRO
2	B	169	GLU
1	A	225	PRO
1	A	156	SER
2	B	170	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	479/499 (96%)	427 (89%)	52 (11%)	6	12
2	B	368/400 (92%)	354 (96%)	14 (4%)	29	54
All	All	847/899 (94%)	781 (92%)	66 (8%)	11	25

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

Mol	Chain	Res	Type
1	A	4	PRO
1	A	6	GLU
1	A	14	PRO
1	A	21	VAL
1	A	52	PRO
1	A	53	GLU
1	A	64	LYS
1	A	70	LYS
1	A	71	TRP
1	A	73	LYS
1	A	97	PRO
1	A	101	LYS
1	A	102	LYS
1	A	104	LYS
1	A	120	LEU
1	A	122	GLU
1	A	123	ASP
1	A	126	LYS
1	A	151	GLN
1	A	182	GLN
1	A	195	ILE
1	A	205	LEU
1	A	248	GLU
1	A	255	ASN
1	A	279	LEU
1	A	295	LEU
1	A	325	LEU
1	A	340	GLN
1	A	344	GLU
1	A	345	PRO
1	A	356	ARG
1	A	358	ARG
1	A	362	THR
1	A	368	LEU
1	A	369	THR
1	A	373	GLN
1	A	386	THR
1	A	396	GLU
1	A	402	TRP
1	A	404	GLU
1	A	423	VAL
1	A	431	LYS

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Mol	Chain	Res	Type
1	A	452	LEU
1	A	458	VAL
1	A	474	ASN
1	A	475	GLN
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	500	GLN
1	A	501	TYR
1	A	533	LEU
2	B	8	VAL
2	B	39	THR
2	B	40	GLU
2	B	73	LYS
2	B	209	LEU
2	B	249	LYS
2	B	280	CYS
2	B	283	LEU
2	B	303	LEU
2	B	323	LYS
2	B	368	LEU
2	B	388	LYS
2	B	425	LEU
2	B	429	LEU

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	182	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	334	GLN
1	A	336	GLN
1	A	361	HIS
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
2	B	145	GLN
2	B	161	GLN
2	B	175	ASN

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Mol	Chain	Res	Type
2	B	182	GLN
2	B	197	GLN
2	B	208	HIS
2	B	255	ASN
2	B	269	GLN
2	B	332	GLN
2	B	336	GLN
2	B	361	HIS
2	B	394	GLN
2	B	418	ASN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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
1	CSD	A	280	1	4,7,8	1.49	1 (25%)	1,8,10	4.47	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	2.64	1.50	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	4.47	113.83	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

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	GWB	A	999	-	21,23,23	2.61	9 (42%)	28,33,33	2.09	5 (17%)

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	GWB	A	999	-	-	0/6/12/12	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	GWB	CC-CB	7.35	1.68	1.45
3	A	999	GWB	C4-C5	4.54	1.40	1.35
3	A	999	GWB	C6-N1	3.50	1.40	1.35
3	A	999	GWB	C6-C5	3.25	1.50	1.43
3	A	999	GWB	C9-C8	2.92	1.42	1.37
3	A	999	GWB	C7-C8	2.61	1.42	1.37
3	A	999	GWB	C3-C2	2.59	1.45	1.41
3	A	999	GWB	C11-C5	2.39	1.55	1.52
3	A	999	GWB	C10-C9	2.12	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	GWB	CD-CC-CB	-6.41	103.97	119.09
3	A	999	GWB	CE-CC-CB	-5.98	104.98	119.09
3	A	999	GWB	O4-C4-C3	3.06	120.60	116.12
3	A	999	GWB	C11-C5-C4	-2.60	118.33	123.81
3	A	999	GWB	C9-C8-C7	-2.12	120.44	123.23

There are no chirality outliers.

There are no torsion outliers.

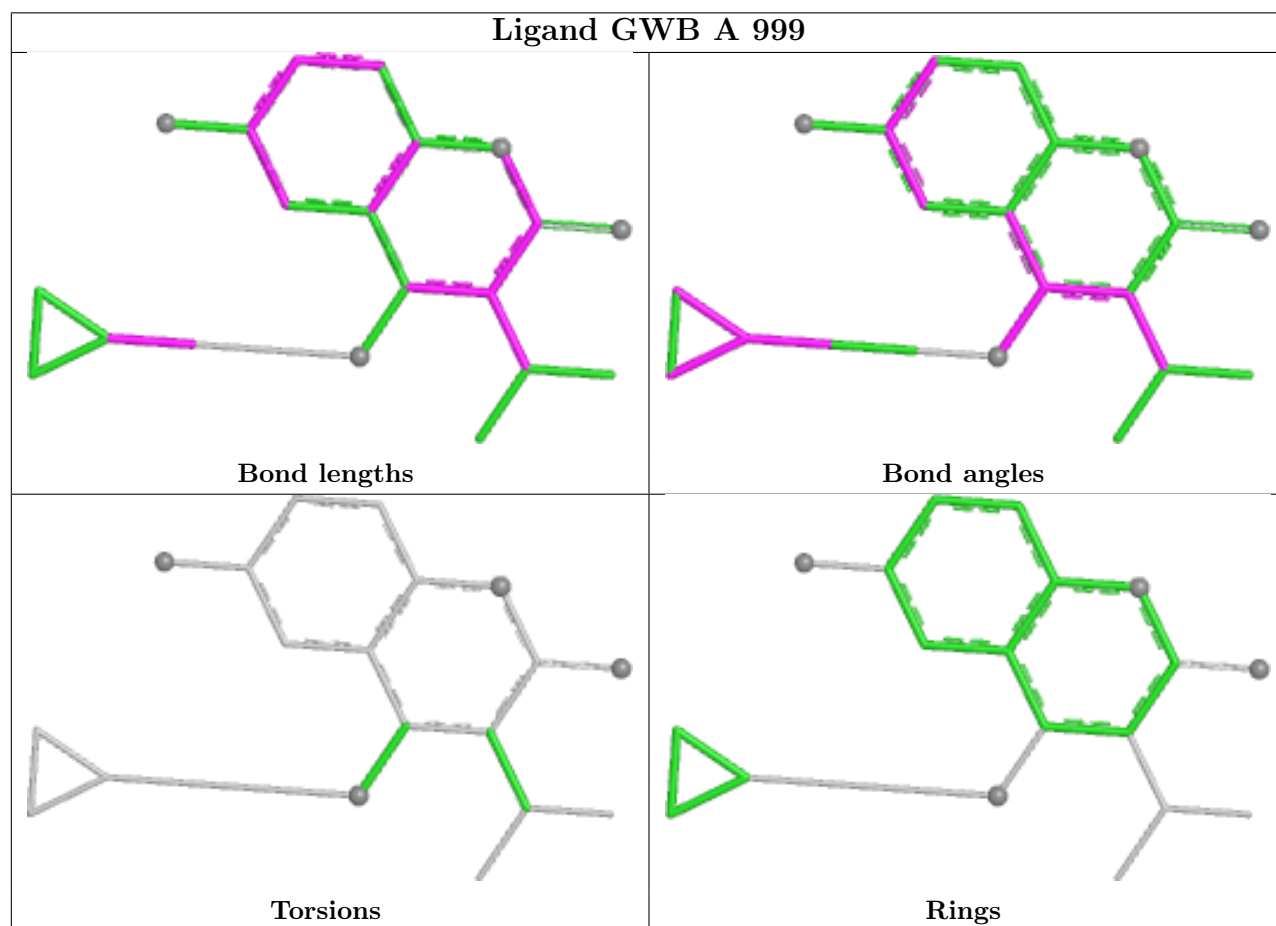
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	GWB	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	534/560 (95%)	-0.32	0 100 100	26, 65, 110, 146	0
2	B	404/440 (91%)	-0.41	3 (0%) 84 80	27, 61, 111, 138	0
All	All	938/1000 (93%)	-0.36	3 (0%) 90 89	26, 63, 111, 146	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	177	ASP	2.4
2	B	435	VAL	2.3
2	B	93	GLY	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	280	8/9	0.96	0.06	52,60,64,66	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

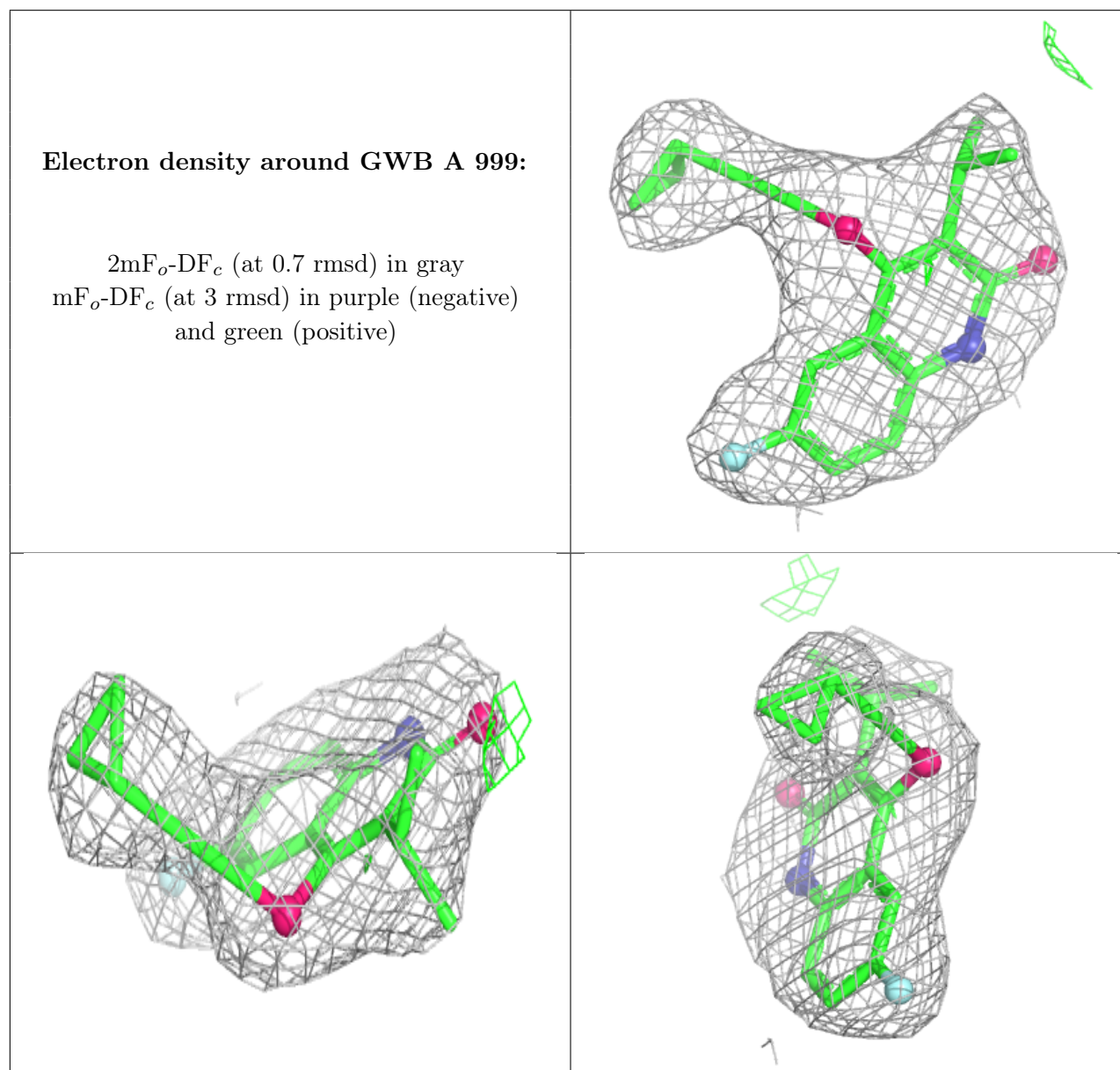
6.4 Ligands [i](#)

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	GWB	A	999	21/21	0.95	0.10	39,45,52,56	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.