



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:08 AM UTC

PDB ID : 1C1B / pdb_00001c1b
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH GCA-186
Authors : Hopkins, A.L.; Ren, J.; Tanaka, H.; Baba, B.; Okamoto, M.; Stuart, D.I.; Stammers, D.K.
Deposited on : 1999-07-21
Resolution : 2.50 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

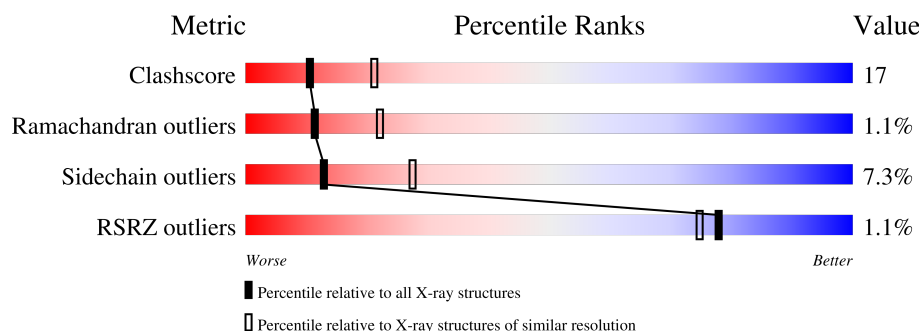
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	% 59% 32% 5% .
2	B	440	2% 60% 30% . 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7888 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 HIV-1 REVERSE TRANSCRIPTASE (A-CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4389	2842	732	807	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

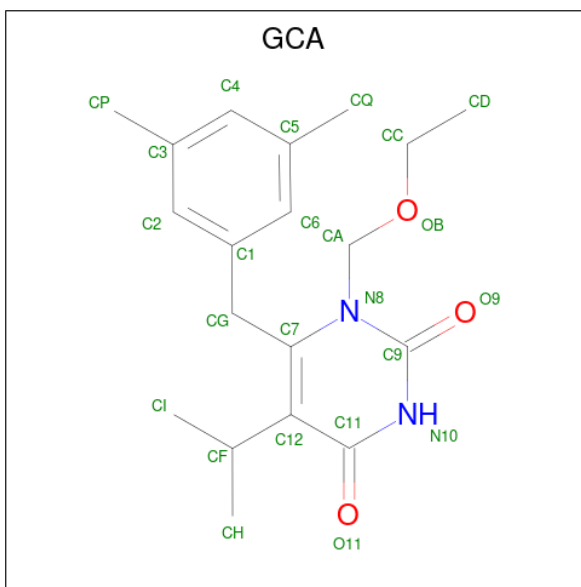
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (B-CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	0	0
			3419	2225	566	621	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	172	LYS	ARG	conflict	UNP P04585
B	428	ASN	GLN	conflict	UNP P04585

- Molecule 3 is 6-(3',5'-DIMETHYLBENZYL)-1-ETHOXYMETHYL-5-ISOPROPYLURACIL (CCD ID: GCA) (formula: C₁₉H₂₆N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	19	2	3		

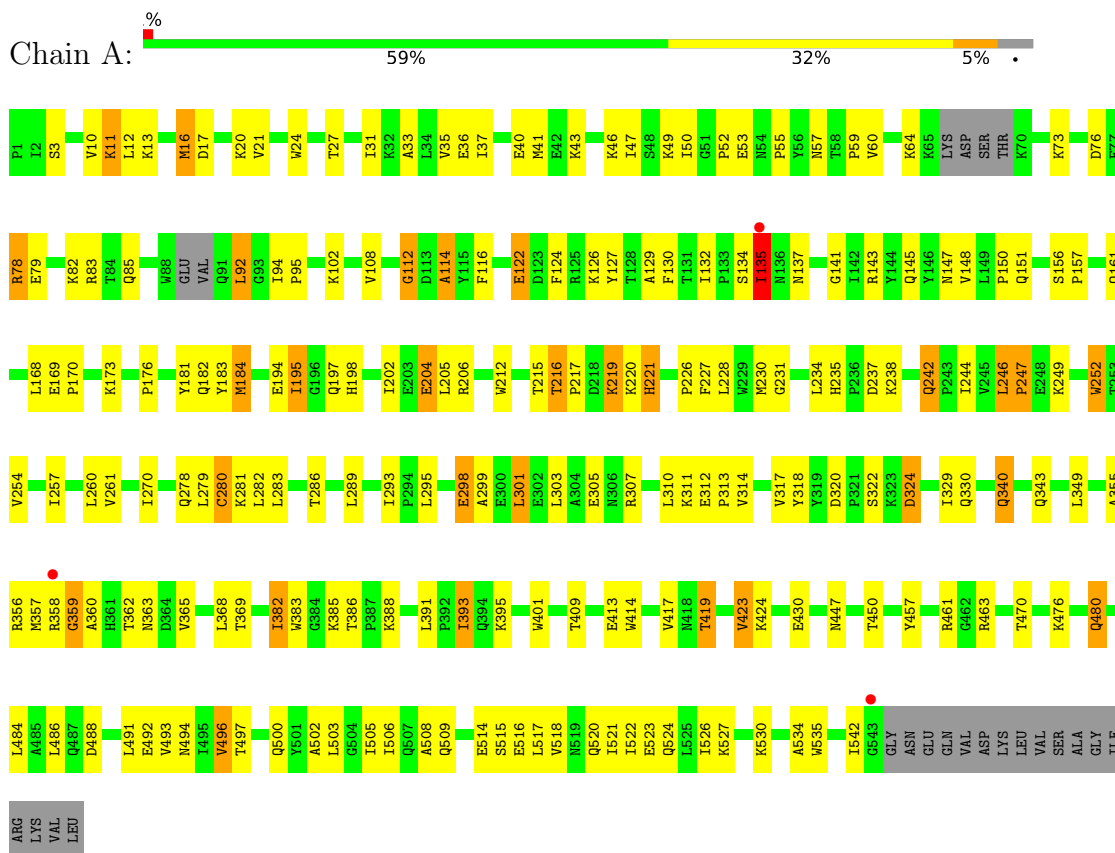
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	40	Total O 40 40	0	0
4	B	16	Total O 16 16	0	0

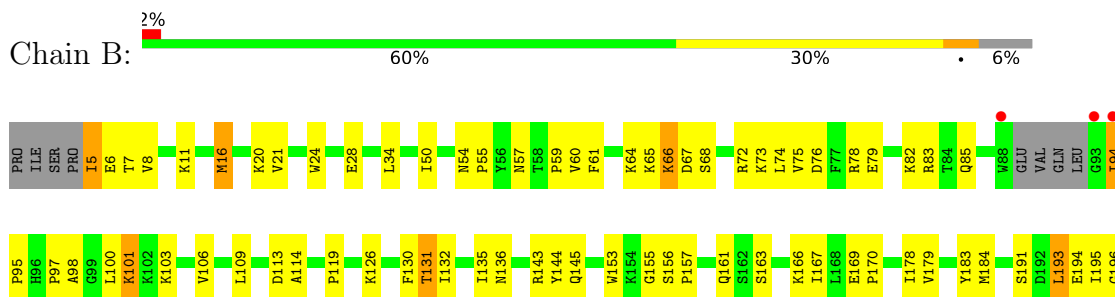
3 Residue-property plots [i](#)

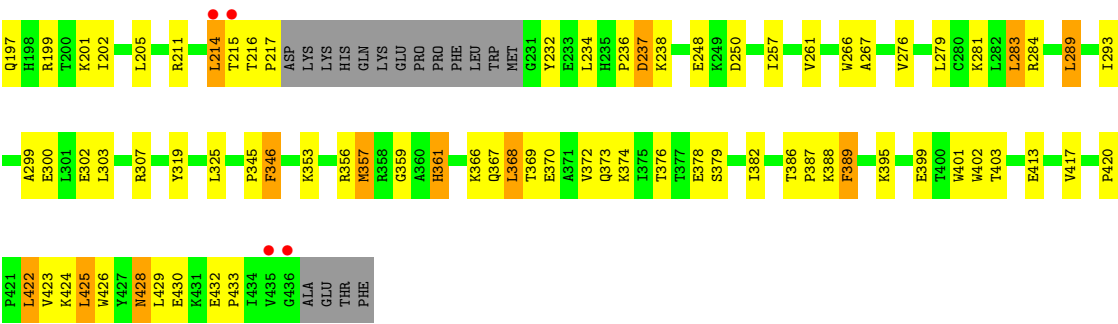
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (A-CHAIN)



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (B-CHAIN)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.00Å 111.50Å 73.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.50) 92.3 (20.00-2.51)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.255 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.6	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	0.96	EDS
Total number of atoms	7888	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: GCA, CSD

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	0/4495	0.95	16/6104 (0.3%)
2	B	0.47	0/3515	0.98	13/4775 (0.3%)
All	All	0.47	0/8010	0.96	29/10879 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	238	LYS	N-CA-C	-11.90	96.55	114.16
2	B	250	ASP	N-CA-C	-8.02	100.89	111.24
1	A	343	GLN	N-CA-C	-6.52	105.21	113.43
2	B	401	TRP	N-CA-C	6.50	123.16	114.12
2	B	131	THR	N-CA-C	6.06	119.01	108.76
1	A	147	ASN	N-CA-C	-6.05	105.19	113.30
1	A	382	ILE	N-CA-C	6.03	116.66	110.82
1	A	388	LYS	N-CA-C	-5.98	99.50	109.24
2	B	417	VAL	N-CA-C	5.95	117.28	108.65
1	A	311	LYS	N-CA-C	-5.87	105.22	112.90
2	B	428	ASN	N-CA-C	-5.70	105.43	112.38
2	B	389	PHE	N-CA-C	5.68	119.50	109.96
2	B	54	ASN	CA-C-N	5.44	126.29	120.47
2	B	54	ASN	C-N-CA	5.44	126.29	120.47
1	A	246	LEU	CA-C-N	5.42	126.62	119.84
1	A	246	LEU	C-N-CA	5.42	126.62	119.84
2	B	402	TRP	N-CA-C	5.42	117.19	111.28
1	A	242	GLN	CA-C-N	5.30	125.60	119.93
1	A	242	GLN	C-N-CA	5.30	125.60	119.93
1	A	204	GLU	N-CA-C	-5.29	105.42	111.14
1	A	349	LEU	N-CA-C	-5.27	105.13	112.45
1	A	252	TRP	N-CA-C	5.25	116.96	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ALA	N-CA-C	-5.22	106.75	113.23
1	A	216	THR	CA-C-N	5.17	126.31	119.84
1	A	216	THR	C-N-CA	5.17	126.31	119.84
2	B	101	LYS	N-CA-C	-5.17	105.77	111.71
1	A	53	GLU	N-CA-C	-5.14	106.84	113.01
2	B	346	PHE	N-CA-CB	-5.10	108.36	114.17
2	B	413	GLU	N-CA-C	-5.02	103.10	110.52

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	4389	0	4436	150	0
2	B	3419	0	3454	118	0
3	A	24	0	26	1	0
4	A	40	0	0	3	0
4	B	16	0	0	0	0
All	All	7888	0	7916	264	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 (264) 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:215:THR:HG22	1:A:216:THR:H	1.29	0.97
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.30	0.92
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.34	0.90
1:A:13:LYS:HB2	1:A:16:MET:HE3	1.56	0.88
1:A:260:LEU:HD23	1:A:279:LEU:HD21	1.55	0.86
1:A:542:ILE:HG23	2:B:283:LEU:HB3	1.58	0.85
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.74	0.85
2:B:236:PRO:O	2:B:237:ASP:HB3	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:LYS:HE2	2:B:430:GLU:HB3	1.57	0.84
1:A:362:THR:HG22	1:A:363:ASN:H	1.43	0.83
1:A:41:MET:HE3	1:A:47:ILE:HD13	1.63	0.81
2:B:66:LYS:HE2	2:B:66:LYS:HA	1.63	0.80
1:A:357:MET:O	1:A:358:ARG:HG2	1.80	0.80
1:A:280:CSD:C	1:A:281:LYS:N	2.44	0.80
1:A:235:HIS:HB2	1:A:238:LYS:O	1.81	0.80
1:A:17:ASP:O	1:A:83:ARG:HD3	1.83	0.79
1:A:215:THR:HG22	1:A:216:THR:N	1.98	0.78
2:B:378:GLU:O	2:B:382:ILE:HG12	1.84	0.76
2:B:357:MET:HE3	2:B:357:MET:HA	1.66	0.76
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.69	0.74
2:B:11:LYS:H	2:B:85:GLN:HE21	1.34	0.74
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.02	0.74
2:B:319:TYR:HE2	2:B:325:LEU:HD11	1.51	0.74
1:A:116:PHE:CE1	1:A:151:GLN:HG2	2.24	0.73
2:B:126:LYS:HA	2:B:145:GLN:HE21	1.54	0.73
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.70	0.72
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.04	0.71
2:B:319:TYR:CE2	2:B:325:LEU:HD11	2.26	0.71
1:A:360:ALA:HA	1:A:514:GLU:HG2	1.74	0.70
1:A:102:LYS:NZ	1:A:237:ASP:HA	2.07	0.69
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.27	0.69
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.74	0.69
2:B:97:PRO:HG2	2:B:100:LEU:HD22	1.75	0.69
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.08	0.68
1:A:13:LYS:HB2	1:A:16:MET:CE	2.24	0.68
1:A:116:PHE:HE1	1:A:151:GLN:HG2	1.57	0.68
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.76	0.68
2:B:79:GLU:O	2:B:83:ARG:HG3	1.94	0.68
1:A:217:PRO:HB2	1:A:221:HIS:CE1	2.29	0.67
1:A:516:GLU:OE1	1:A:516:GLU:HA	1.94	0.67
2:B:214:LEU:H	2:B:214:LEU:HD23	1.60	0.66
1:A:215:THR:CG2	1:A:216:THR:H	2.05	0.66
1:A:41:MET:HE1	1:A:73:LYS:HE3	1.77	0.65
1:A:60:VAL:HG21	1:A:130:PHE:CD1	2.32	0.65
2:B:426:TRP:O	2:B:429:LEU:HB2	1.96	0.64
2:B:366:LYS:O	2:B:370:GLU:HG3	1.97	0.64
2:B:97:PRO:HG2	2:B:100:LEU:CD2	2.27	0.64
1:A:228:LEU:HD21	1:A:242:GLN:CD	2.22	0.64
2:B:215:THR:O	2:B:217:PRO:HD3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:NZ	1:A:11:LYS:HB3	2.14	0.62
2:B:359:GLY:HA2	2:B:361:HIS:CE1	2.33	0.62
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.80	0.62
1:A:11:LYS:O	1:A:85:GLN:HB3	1.98	0.62
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.47	0.62
1:A:217:PRO:HB2	1:A:221:HIS:HE1	1.64	0.61
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.30	0.61
1:A:31:ILE:O	1:A:35:VAL:HG23	1.99	0.61
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.15	0.61
2:B:199:ARG:O	2:B:202:ILE:HB	2.01	0.61
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.35	0.61
1:A:92:LEU:N	1:A:92:LEU:HD13	2.16	0.61
2:B:50:ILE:HD13	2:B:145:GLN:HB2	1.82	0.61
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.83	0.61
2:B:64:LYS:HB2	2:B:64:LYS:NZ	2.16	0.61
1:A:516:GLU:O	1:A:520:GLN:HG2	2.01	0.60
2:B:66:LYS:O	2:B:67:ASP:HB3	2.01	0.60
2:B:163:SER:O	2:B:167:ILE:HG13	2.01	0.60
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.02	0.60
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.85	0.59
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.17	0.58
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.10	0.58
2:B:257:ILE:HB	2:B:283:LEU:HD11	1.84	0.58
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.33	0.58
1:A:3:SER:HB3	1:A:212:TRP:O	2.04	0.58
1:A:184:MET:HE3	1:A:184:MET:HA	1.87	0.57
2:B:432:GLU:HB3	2:B:433:PRO:HD2	1.85	0.57
1:A:40:GLU:O	1:A:43:LYS:HG2	2.05	0.57
2:B:395:LYS:HG2	2:B:399:GLU:OE2	2.05	0.57
2:B:184:MET:HE2	2:B:184:MET:HA	1.87	0.57
1:A:219:LYS:H	1:A:219:LYS:CD	2.19	0.56
1:A:480:GLN:C	1:A:480:GLN:HE21	2.14	0.56
2:B:279:LEU:HD23	2:B:299:ALA:HB1	1.88	0.56
1:A:317:VAL:HG22	1:A:318:TYR:H	1.71	0.56
2:B:66:LYS:C	2:B:68:SER:H	2.14	0.56
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.40	0.55
2:B:16:MET:HG2	2:B:83:ARG:HB3	1.88	0.55
2:B:100:LEU:HD23	2:B:100:LEU:H	1.69	0.55
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.88	0.55
2:B:345:PRO:O	2:B:346:PHE:HB2	2.06	0.55
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLN:OE1	1:A:500:GLN:HA	2.05	0.55
2:B:379:SER:CB	2:B:387:PRO:HD3	2.37	0.55
1:A:417:VAL:HG13	1:A:419:THR:HG22	1.89	0.55
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.89	0.55
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.89	0.54
1:A:102:LYS:HZ2	1:A:237:ASP:HA	1.72	0.54
2:B:5:ILE:HG13	2:B:6:GLU:N	2.22	0.54
1:A:278:GLN:CG	1:A:298:GLU:HB3	2.37	0.54
2:B:74:LEU:HD12	2:B:75:VAL:N	2.22	0.54
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.89	0.54
3:A:999:GCA:HH3	3:A:999:GCA:HG2	1.90	0.54
2:B:368:LEU:O	2:B:372:VAL:HG23	2.08	0.54
1:A:260:LEU:CD2	1:A:279:LEU:HD21	2.33	0.53
2:B:281:LYS:HD3	2:B:284:ARG:NH2	2.23	0.53
2:B:425:LEU:O	2:B:429:LEU:HD13	2.08	0.53
2:B:85:GLN:O	2:B:85:GLN:HG3	2.08	0.53
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.91	0.53
1:A:226:PRO:HB3	1:A:235:HIS:HD2	1.72	0.53
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.73	0.53
1:A:102:LYS:HZ1	1:A:237:ASP:HA	1.73	0.53
2:B:236:PRO:O	2:B:237:ASP:CB	2.49	0.53
1:A:514:GLU:HG3	1:A:515:SER:N	2.24	0.52
2:B:359:GLY:HA2	2:B:361:HIS:NE2	2.24	0.52
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.91	0.52
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.40	0.52
2:B:395:LYS:O	2:B:399:GLU:HG3	2.09	0.52
1:A:206:ARG:HG3	1:A:216:THR:HG21	1.93	0.51
1:A:195:ILE:HD13	1:A:195:ILE:N	2.25	0.51
1:A:270:ILE:HG21	1:A:314:VAL:HG21	1.93	0.51
2:B:424:LYS:O	2:B:428:ASN:HB2	2.10	0.51
1:A:228:LEU:HD11	1:A:242:GLN:HE22	1.76	0.51
2:B:214:LEU:HD23	2:B:214:LEU:N	2.25	0.51
1:A:355:ALA:O	1:A:356:ARG:HD3	2.11	0.51
1:A:463:ARG:NH1	1:A:488:ASP:O	2.44	0.51
1:A:486:LEU:HD13	1:A:524:GLN:HB3	1.93	0.51
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.45	0.50
1:A:317:VAL:HG22	1:A:318:TYR:N	2.26	0.50
1:A:122:GLU:H	1:A:122:GLU:CD	2.19	0.50
1:A:244:ILE:HB	1:A:310:LEU:HD13	1.93	0.50
1:A:480:GLN:O	1:A:480:GLN:NE2	2.45	0.50
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LYS:HA	2:B:145:GLN:NE2	2.25	0.50
1:A:78:ARG:O	1:A:82:LYS:HG3	2.11	0.50
1:A:204:GLU:HG2	4:A:1049:HOH:O	2.11	0.50
2:B:195:ILE:O	2:B:199:ARG:HG3	2.11	0.50
1:A:231:GLY:HA2	1:A:242:GLN:NE2	2.27	0.50
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.93	0.50
1:A:324:ASP:OD2	1:A:324:ASP:N	2.45	0.50
2:B:237:ASP:O	2:B:237:ASP:CG	2.54	0.50
2:B:276:VAL:HA	2:B:302:GLU:OE2	2.12	0.50
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.47	0.49
1:A:503:LEU:HD21	2:B:422:LEU:HD22	1.94	0.49
1:A:522:ILE:O	1:A:526:ILE:HG13	2.12	0.49
2:B:109:LEU:HD23	2:B:216:THR:HG21	1.94	0.49
1:A:228:LEU:HD21	1:A:242:GLN:NE2	2.27	0.49
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.95	0.49
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.56	0.49
2:B:103:LYS:HD2	2:B:191:SER:HA	1.95	0.49
1:A:497:THR:O	1:A:535:TRP:HA	2.12	0.49
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.95	0.49
1:A:11:LYS:HB3	1:A:11:LYS:HZ3	1.77	0.48
1:A:383:TRP:O	1:A:385:LYS:HG3	2.13	0.48
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.43	0.48
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.49	0.48
2:B:61:PHE:CE2	2:B:74:LEU:HG	2.48	0.48
2:B:100:LEU:HD23	2:B:100:LEU:N	2.27	0.48
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.43	0.48
1:A:365:VAL:O	1:A:369:THR:HG23	2.13	0.48
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.94	0.48
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.96	0.48
2:B:94:ILE:HD12	2:B:95:PRO:HD2	1.95	0.47
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.45	0.47
2:B:106:VAL:HB	2:B:234:LEU:HB2	1.96	0.47
1:A:523:GLU:O	1:A:527:LYS:HD3	2.14	0.47
1:A:132:ILE:O	1:A:141:GLY:HA3	2.15	0.47
1:A:362:THR:HG22	1:A:363:ASN:N	2.20	0.47
2:B:211:ARG:O	2:B:211:ARG:HD3	2.15	0.46
2:B:215:THR:C	2:B:217:PRO:HD3	2.41	0.46
1:A:134:SER:O	1:A:135:ILE:C	2.58	0.46
2:B:156:SER:HB2	2:B:157:PRO:CD	2.45	0.46
1:A:382:ILE:O	2:B:136:ASN:HB2	2.16	0.46
1:A:161:GLN:NE2	1:A:182:GLN:NE2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LYS:O	1:A:480:GLN:HB2	2.16	0.46
1:A:228:LEU:HA	1:A:228:LEU:HD22	1.82	0.46
1:A:148:VAL:O	1:A:150:PRO:HD3	2.16	0.45
1:A:37:ILE:O	1:A:40:GLU:HB3	2.16	0.45
1:A:17:ASP:O	1:A:83:ARG:CD	2.60	0.45
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.81	0.45
2:B:281:LYS:HD3	2:B:284:ARG:CZ	2.46	0.45
2:B:94:ILE:HA	2:B:95:PRO:HD3	1.86	0.45
2:B:100:LEU:CD2	2:B:100:LEU:H	2.29	0.45
1:A:457:TYR:CD1	1:A:457:TYR:C	2.94	0.45
2:B:425:LEU:HD12	2:B:425:LEU:HA	1.83	0.45
1:A:254:VAL:HG22	1:A:286:THR:HG21	1.99	0.45
2:B:65:LYS:O	2:B:68:SER:HB3	2.17	0.45
1:A:542:ILE:O	1:A:542:ILE:HG22	2.16	0.45
1:A:502:ALA:O	1:A:506:ILE:HG13	2.16	0.45
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.81	0.44
1:A:194:GLU:O	1:A:195:ILE:C	2.60	0.44
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.32	0.44
1:A:413:GLU:HG3	4:A:1014:HOH:O	2.15	0.44
1:A:20:LYS:HZ1	1:A:55:PRO:HB2	1.82	0.44
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.53	0.44
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.17	0.44
2:B:132:ILE:HD12	2:B:132:ILE:N	2.32	0.44
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.06	0.44
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.17	0.44
2:B:11:LYS:HE3	2:B:11:LYS:HB2	1.76	0.44
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.99	0.44
2:B:357:MET:HA	2:B:357:MET:CE	2.41	0.44
2:B:359:GLY:C	2:B:361:HIS:H	2.25	0.44
2:B:195:ILE:HG23	2:B:196:GLY:N	2.33	0.44
1:A:492:GLU:HA	1:A:530:LYS:O	2.17	0.44
2:B:178:ILE:CD1	2:B:201:LYS:HG2	2.47	0.44
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.53	0.44
1:A:283:LEU:O	1:A:286:THR:HG23	2.18	0.43
1:A:280:CSD:O	1:A:281:LYS:N	2.51	0.43
2:B:34:LEU:HD21	2:B:73:LYS:HG3	2.00	0.43
1:A:198:HIS:O	1:A:202:ILE:HG12	2.19	0.43
2:B:57:ASN:ND2	2:B:143:ARG:HH11	2.14	0.43
1:A:320:ASP:OD2	1:A:322:SER:OG	2.37	0.43
2:B:109:LEU:HG	2:B:216:THR:HG22	2.00	0.43
2:B:72:ARG:HG3	2:B:72:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:VAL:HA	1:A:534:ALA:O	2.18	0.43
2:B:183:TYR:O	2:B:184:MET:HB2	2.17	0.43
1:A:417:VAL:HG13	1:A:417:VAL:O	2.19	0.43
1:A:64:LYS:HB3	1:A:64:LYS:HE2	1.82	0.43
1:A:330:GLN:OE1	1:A:340:GLN:OE1	2.37	0.43
1:A:357:MET:C	1:A:359:GLY:H	2.27	0.43
2:B:178:ILE:HD11	2:B:201:LYS:HG2	2.00	0.43
1:A:254:VAL:HG22	1:A:293:ILE:HD11	2.00	0.43
1:A:503:LEU:HD21	2:B:422:LEU:CD2	2.48	0.43
1:A:46:LYS:HE3	1:A:116:PHE:O	2.19	0.42
1:A:33:ALA:O	1:A:36:GLU:HB3	2.19	0.42
2:B:136:ASN:CG	2:B:136:ASN:O	2.62	0.42
1:A:169:GLU:N	1:A:170:PRO:HD2	2.34	0.42
2:B:5:ILE:CG1	2:B:6:GLU:N	2.78	0.42
1:A:508:ALA:O	1:A:509:GLN:C	2.63	0.42
2:B:78:ARG:O	2:B:82:LYS:HG3	2.19	0.42
2:B:11:LYS:N	2:B:85:GLN:HE21	2.09	0.42
1:A:10:VAL:HG12	1:A:124:PHE:CD1	2.54	0.42
1:A:27:THR:O	1:A:31:ILE:HG13	2.19	0.42
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.86	0.42
2:B:98:ALA:O	2:B:101:LYS:HG2	2.19	0.42
1:A:430:GLU:HG2	4:A:1018:HOH:O	2.19	0.42
1:A:362:THR:CG2	1:A:363:ASN:H	2.24	0.42
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.54	0.42
2:B:11:LYS:O	2:B:85:GLN:HG2	2.19	0.42
1:A:194:GLU:O	1:A:197:GLN:N	2.53	0.41
1:A:116:PHE:HE1	1:A:151:GLN:CG	2.29	0.41
1:A:312:GLU:OE1	1:A:313:PRO:HD2	2.20	0.41
2:B:376:THR:CG2	2:B:386:THR:HG22	2.50	0.41
1:A:282:LEU:HD21	1:A:299:ALA:HB2	2.02	0.41
1:A:173:LYS:O	1:A:176:PRO:HD3	2.20	0.41
1:A:301:LEU:O	1:A:305:GLU:HG3	2.21	0.41
1:A:480:GLN:HE22	1:A:484:LEU:HG	1.86	0.41
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.03	0.41
1:A:219:LYS:O	1:A:220:LYS:C	2.63	0.41
1:A:257:ILE:O	1:A:261:VAL:HG23	2.21	0.41
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.51	0.41
2:B:66:LYS:C	2:B:68:SER:N	2.79	0.41
2:B:194:GLU:HG3	2:B:196:GLY:H	1.85	0.41
1:A:112:GLY:C	1:A:114:ALA:H	2.28	0.41
1:A:57:ASN:HA	1:A:129:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.87	0.40
2:B:64:LYS:HB2	2:B:64:LYS:HZ2	1.84	0.40
1:A:252:TRP:NE1	1:A:295:LEU:HD11	2.37	0.40
2:B:61:PHE:CD1	2:B:403:THR:HB	2.56	0.40
1:A:298:GLU:N	1:A:298:GLU:OE1	2.54	0.40
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.55	0.40
1:A:12:LEU:HD22	1:A:83:ARG:HB3	2.03	0.40
1:A:49:LYS:HA	1:A:143:ARG:O	2.21	0.40
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.57	0.40
2:B:356:ARG:HB2	2:B:367:GLN:HG2	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	529/560 (94%)	485 (92%)	38 (7%)	6 (1%)	11	22
2	B	409/440 (93%)	377 (92%)	28 (7%)	4 (1%)	12	24
All	All	938/1000 (94%)	862 (92%)	66 (7%)	10 (1%)	11	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	193	LEU
2	B	237	ASP
1	A	112	GLY
1	A	135	ILE
2	B	232	TYR
1	A	359	GLY
2	B	361	HIS
1	A	247	PRO

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Mol	Chain	Res	Type
1	A	16	MET
1	A	52	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%)	443 (92%)	36 (8%)	12	26
2	B	376/400 (94%)	350 (93%)	26 (7%)	14	30
All	All	855/899 (95%)	793 (93%)	62 (7%)	13	27

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	24	TRP
1	A	78	ARG
1	A	92	LEU
1	A	108	VAL
1	A	122	GLU
1	A	135	ILE
1	A	137	ASN
1	A	168	LEU
1	A	184	MET
1	A	195	ILE
1	A	205	LEU
1	A	219	LYS
1	A	221	HIS
1	A	230	MET
1	A	249	LYS
1	A	289	LEU
1	A	298	GLU
1	A	301	LEU
1	A	303	LEU
1	A	324	ASP

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Mol	Chain	Res	Type
1	A	340	GLN
1	A	368	LEU
1	A	386	THR
1	A	393	ILE
1	A	419	THR
1	A	423	VAL
1	A	424	LYS
1	A	461	ARG
1	A	470	THR
1	A	480	GLN
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	505	ILE
1	A	517	LEU
2	B	5	ILE
2	B	8	VAL
2	B	16	MET
2	B	20	LYS
2	B	24	TRP
2	B	55	PRO
2	B	66	LYS
2	B	94	ILE
2	B	113	ASP
2	B	161	GLN
2	B	166	LYS
2	B	179	VAL
2	B	197	GLN
2	B	205	LEU
2	B	214	LEU
2	B	283	LEU
2	B	289	LEU
2	B	293	ILE
2	B	300	GLU
2	B	303	LEU
2	B	357	MET
2	B	368	LEU
2	B	374	LYS
2	B	388	LYS
2	B	422	LEU
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	151	GLN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	235	HIS
1	A	242	GLN
1	A	330	GLN
1	A	332	GLN
1	A	361	HIS
1	A	480	GLN
1	A	487	GLN
1	A	512	GLN
2	B	57	ASN
2	B	85	GLN
2	B	145	GLN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	255	ASN
2	B	278	GLN
2	B	373	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	1.91	1 (25%)	1,8,10	6.14	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	-	1/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	3.58	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	6.14	116.91	105.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	2	0

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	GCA	A	999	-	25,25,25	1.75	4 (16%)	28,35,35	1.02	2 (7%)

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	GCA	A	999	-	-	1/12/12/12	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	GCA	C7-C12	6.31	1.42	1.35
3	A	999	GCA	CG-C7	3.41	1.54	1.50
3	A	999	GCA	CA-N8	2.34	1.50	1.46
3	A	999	GCA	CF-C12	2.17	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	GCA	C1-CG-C7	2.98	120.77	114.78
3	A	999	GCA	CF-C12-C7	2.40	126.51	120.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	GCA	N8-CA-OB-CC

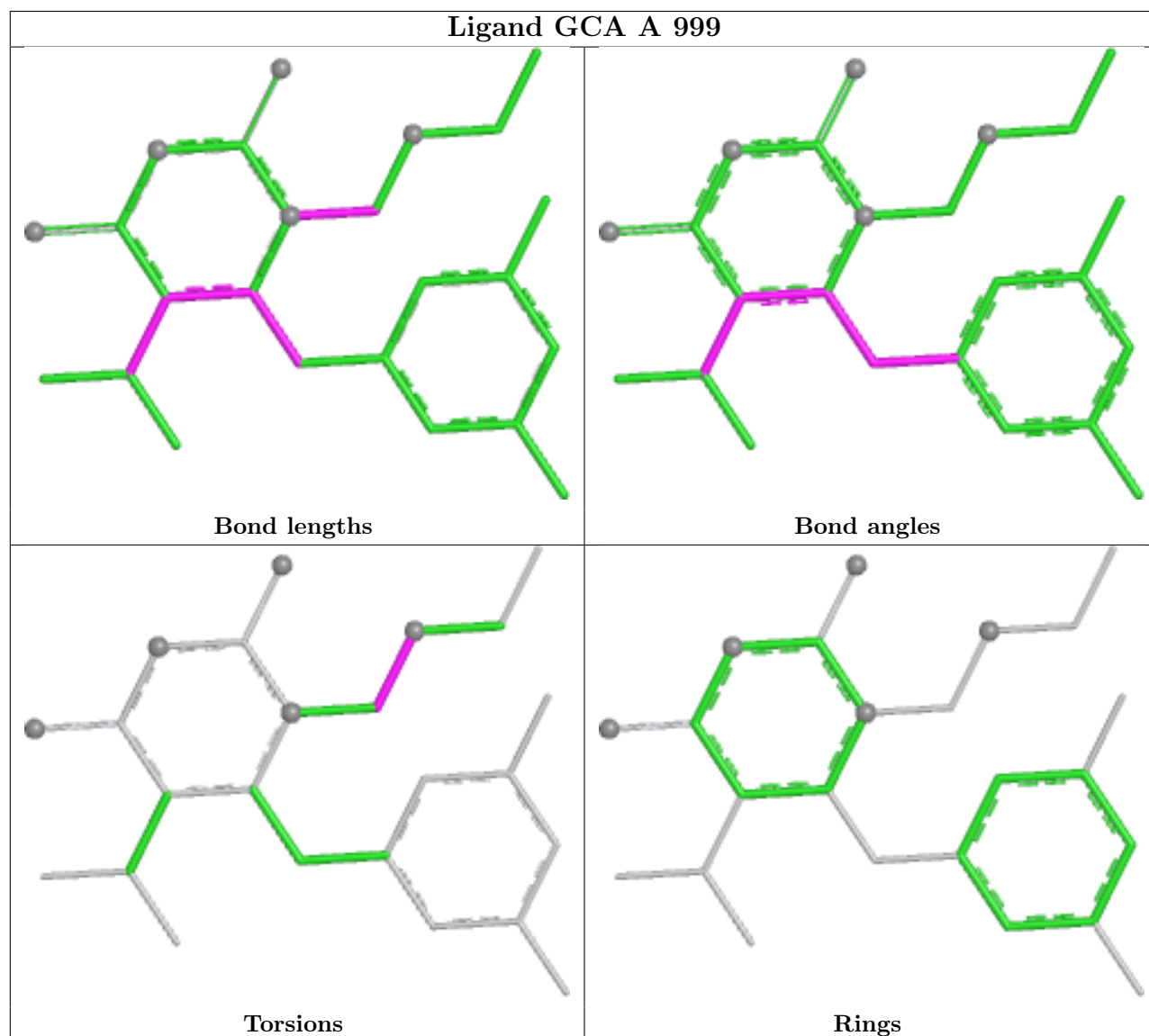
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	GCA	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	280:CSD	C	281:LYS	N	2.44

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	536/560 (95%)	-0.40	3 (0%) 85 83	20, 52, 109, 150	0
2	B	415/440 (94%)	-0.37	7 (1%) 69 65	18, 50, 111, 145	0
All	All	951/1000 (95%)	-0.39	10 (1%) 78 75	18, 51, 111, 150	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	435	VAL	3.3
2	B	88	TRP	3.2
2	B	214	LEU	3.0
1	A	543	GLY	3.0
2	B	436	GLY	2.8
2	B	215	THR	2.3
1	A	358	ARG	2.3
1	A	135	ILE	2.3
2	B	94	ILE	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	0.90	0.09	43,52,66,67	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

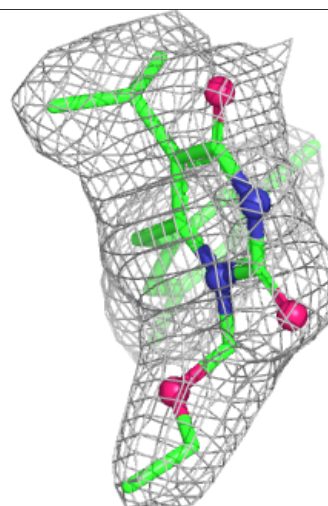
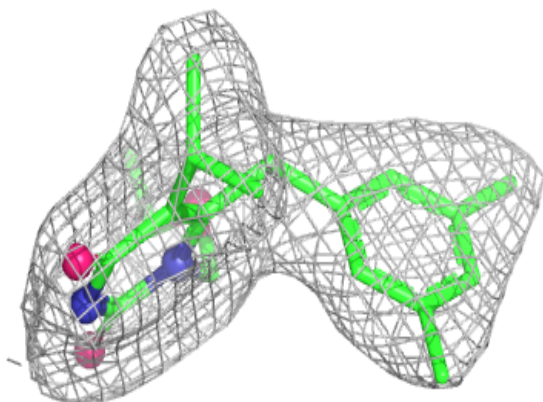
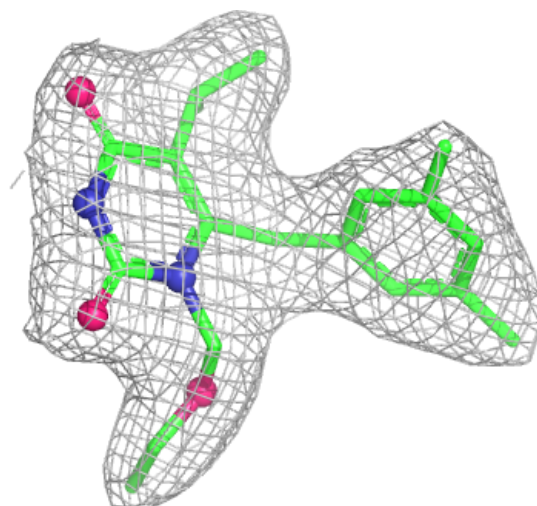
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GCA	A	999	24/24	0.97	0.06	13,29,39,40	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 GCA A 999:

$2mF_o-DF_c$ (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.