



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:44 am BST

PDB ID : 1KLM
Title : HIV-1 REVERSE TRANSCRIPTASE COMPLEXED WITH BHAP U-90152
Authors : Ren, J.; Esnouf, R.M.; Stammers, D.K.; Stuart, D.I.
Deposited on : 1997-03-17
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

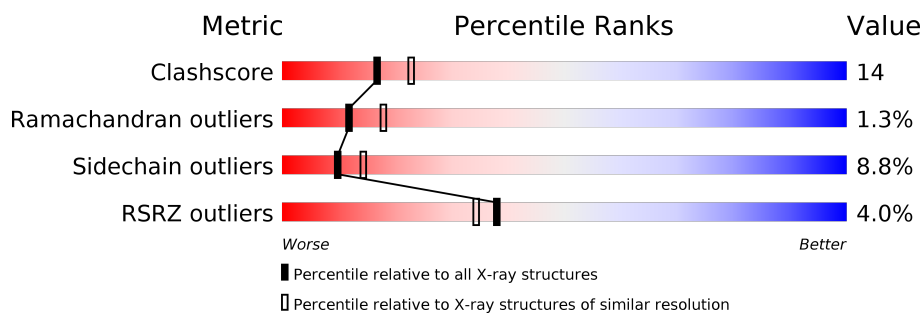
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on 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 4 unique types of molecules in this entry. The entry contains 7865 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4403	2848	733	814	8			

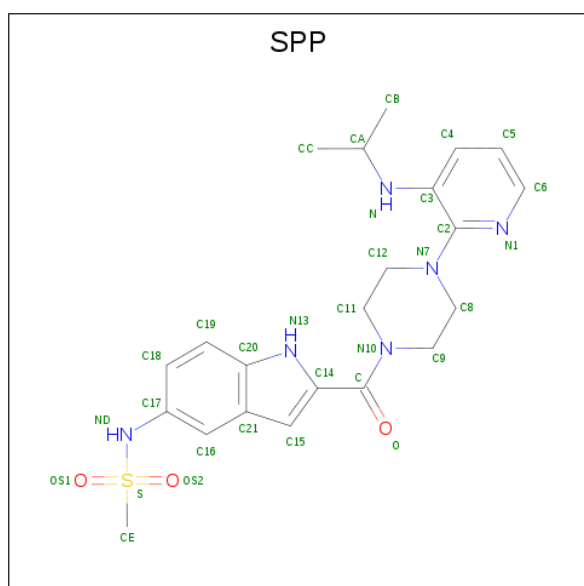
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3358	2183	558	610	7			

- Molecule 3 is (1-(5-METHANSULPHONAMIDO-1H-INDOL-2-YL-CARBONYL)4-[METHYLAMINO]PYRIDINYL)PIPERAZINE (three-letter code: SPP) (formula: C₂₂H₂₈N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	22	6	3	1		

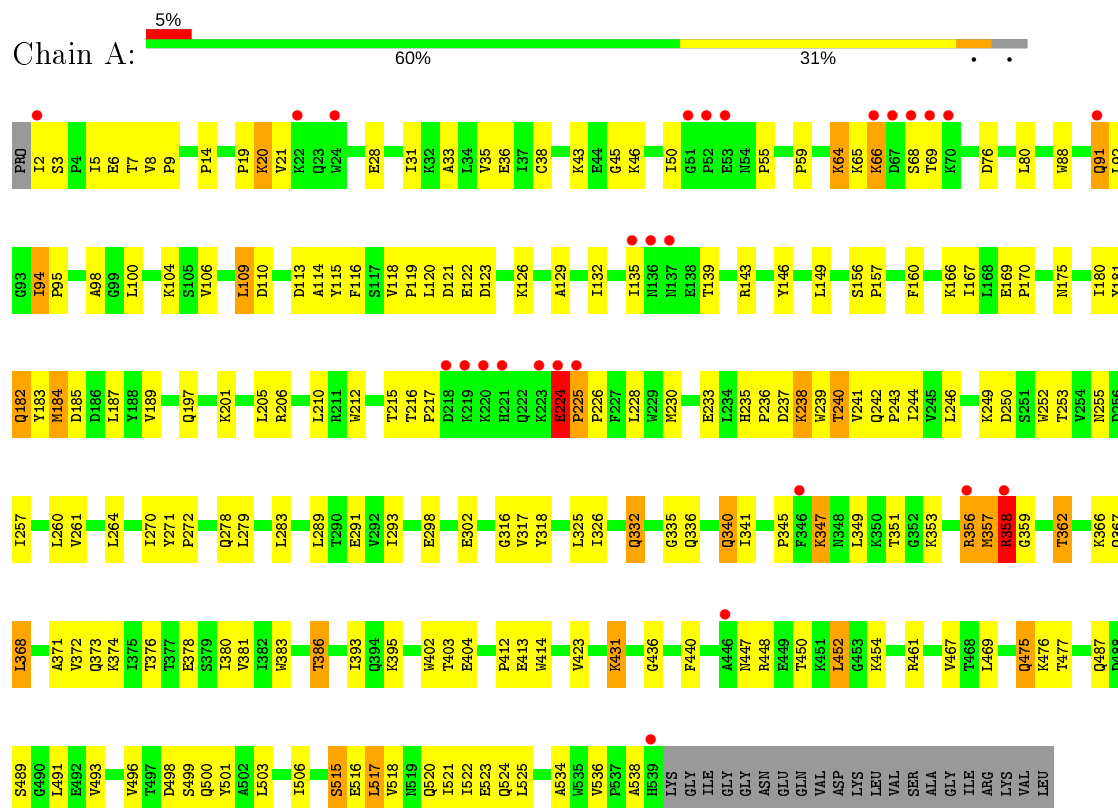
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	32	Total	O	0	0
			32	32		

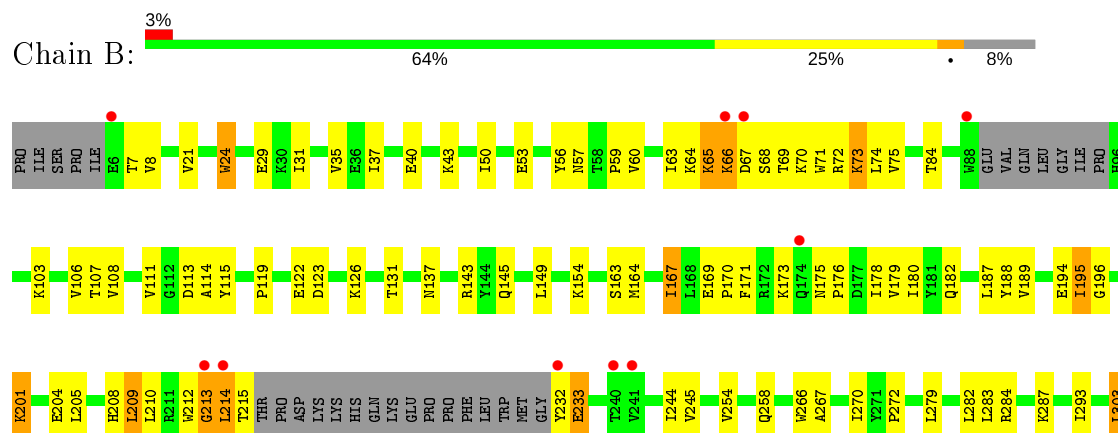
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.80 Å 109.40 Å 72.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 19.84 – 2.65	Depositor EDS
% Data completeness (in resolution range)	86.8 (20.00-2.65) 87.3 (19.84-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.67 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.237 , 0.313 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7865	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: SPP, 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	0.34	0/4511	0.61	1/6132 (0.0%)
2	B	0.34	0/3452	0.61	0/4687
All	All	0.34	0/7963	0.61	1/10819 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLU	N-CA-C	5.51	125.88	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4403	0	4444	134	0
2	B	3358	0	3384	85	0
3	A	32	0	28	10	0
4	A	40	0	0	0	0
4	B	32	0	0	0	0
All	All	7865	0	7856	221	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 14.

All (221) 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:216:THR:HB	1:A:217:PRO:HD2	1.27	1.16
1:A:225:PRO:HB2	1:A:226:PRO:HD2	1.59	0.84
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.68	0.76
1:A:358:ARG:HD2	1:A:358:ARG:O	1.86	0.76
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.68	0.75
1:A:335:GLY:HA2	1:A:367:GLN:OE1	1.87	0.74
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.67	0.74
2:B:213:GLY:C	2:B:214:LEU:HD23	2.09	0.73
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.24	0.72
2:B:84:THR:HB	2:B:154:LYS:HE2	1.71	0.72
1:A:216:THR:CB	1:A:217:PRO:HD2	2.13	0.71
1:A:2:ILE:HG22	1:A:3:SER:H	1.55	0.70
1:A:216:THR:HB	1:A:217:PRO:CD	2.16	0.70
1:A:33:ALA:O	1:A:36:GLU:HG2	1.91	0.70
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.76	0.68
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.75	0.68
3:A:999:SPP:C15	3:A:999:SPP:H112	2.23	0.67
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.78	0.66
1:A:64:LYS:H	1:A:64:LYS:HD2	1.61	0.66
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.78	0.65
1:A:516:GLU:O	1:A:520:GLN:HG3	1.96	0.65
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.78	0.64
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.77	0.64
1:A:98:ALA:HB1	1:A:383:TRP:HZ2	1.63	0.64
2:B:214:LEU:N	2:B:214:LEU:HD23	2.13	0.63
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.80	0.63
1:A:238:LYS:HB2	1:A:316:GLY:O	2.00	0.61
1:A:356:ARG:HD2	1:A:356:ARG:O	1.99	0.61
2:B:287:LYS:HE2	2:B:293:ILE:HD11	1.82	0.61
1:A:9:PRO:HG2	2:B:53:GLU:HG3	1.82	0.61
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.66	0.60
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.98	0.60
2:B:270:ILE:O	2:B:272:PRO:HD3	2.00	0.60
1:A:376:THR:O	1:A:380:ILE:HG12	2.01	0.60
1:A:46:LYS:HD3	1:A:116:PHE:HB3	1.84	0.60
1:A:335:GLY:C	1:A:356:ARG:HB3	2.23	0.59
1:A:91:GLN:NE2	1:A:95:PRO:HD3	2.18	0.59
1:A:235:HIS:ND1	1:A:238:LYS:HE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:HE22	1:A:95:PRO:HD3	1.67	0.58
2:B:106:VAL:O	2:B:233:GLU:HB2	2.04	0.58
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.39	0.57
3:A:999:SPP:H15	3:A:999:SPP:H112	1.87	0.57
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.19	0.57
1:A:31:ILE:O	1:A:35:VAL:HG23	2.05	0.57
1:A:225:PRO:HB2	1:A:226:PRO:CD	2.33	0.56
1:A:94:ILE:H	1:A:94:ILE:HD13	1.71	0.56
1:A:109:LEU:HD11	1:A:206:ARG:HH21	1.70	0.56
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.41	0.56
1:A:225:PRO:CB	1:A:226:PRO:HD2	2.33	0.56
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.86	0.55
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.40	0.55
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.41	0.55
2:B:244:ILE:HG13	2:B:426:TRP:CH2	2.41	0.55
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.88	0.55
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.88	0.55
2:B:173:LYS:O	2:B:176:PRO:HD3	2.07	0.55
1:A:106:VAL:HG21	3:A:999:SPP:H121	1.88	0.54
2:B:379:SER:CB	2:B:387:PRO:HD3	2.37	0.54
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.43	0.54
1:A:33:ALA:HA	1:A:36:GLU:OE2	2.08	0.54
1:A:3:SER:OG	1:A:5:ILE:HG22	2.08	0.54
1:A:228:LEU:CD2	1:A:233:GLU:HG2	2.39	0.53
1:A:358:ARG:HH11	1:A:358:ARG:N	2.05	0.53
2:B:267:ALA:HB2	2:B:426:TRP:NE1	2.24	0.53
2:B:64:LYS:HZ2	2:B:69:THR:HA	1.74	0.53
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.89	0.53
2:B:245:VAL:HG13	2:B:431:LYS:HB2	1.91	0.52
2:B:426:TRP:O	2:B:429:LEU:HB2	2.09	0.52
2:B:163:SER:O	2:B:167:ILE:HG22	2.09	0.52
1:A:2:ILE:HD11	1:A:45:GLY:O	2.10	0.52
3:A:999:SPP:H4	3:A:999:SPP:HB2	1.90	0.52
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.90	0.52
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.43	0.52
1:A:28:GLU:HA	1:A:135:ILE:HD11	1.91	0.52
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.92	0.51
1:A:368:LEU:O	1:A:372:VAL:HG23	2.11	0.51
1:A:98:ALA:HB2	1:A:349:LEU:O	2.10	0.51
2:B:114:ALA:HB2	2:B:214:LEU:CD1	2.41	0.51
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.92	0.51
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.93	0.51
1:A:378:GLU:O	1:A:381:VAL:HG12	2.11	0.51
2:B:113:ASP:HB2	2:B:214:LEU:HB3	1.93	0.51
1:A:524:GLN:HA	1:A:524:GLN:HE21	1.76	0.50
1:A:135:ILE:O	1:A:135:ILE:HG22	2.11	0.50
2:B:114:ALA:HB2	2:B:214:LEU:HD11	1.92	0.50
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.47	0.49
1:A:116:PHE:CE1	1:A:146:TYR:HE2	2.31	0.49
2:B:65:LYS:HD3	2:B:72:ARG:HD2	1.93	0.49
1:A:182:GLN:HG2	1:A:187:LEU:CD2	2.42	0.49
1:A:167:ILE:HG23	1:A:212:TRP:CD1	2.48	0.49
2:B:308:GLU:O	2:B:311:LYS:HB2	2.13	0.48
1:A:110:ASP:H	1:A:217:PRO:HD3	1.77	0.48
2:B:64:LYS:NZ	2:B:69:THR:HA	2.28	0.48
2:B:365:VAL:O	2:B:369:THR:HG23	2.13	0.48
1:A:293:ILE:HD12	1:A:293:ILE:N	2.29	0.48
1:A:515:SER:OG	1:A:518:VAL:HG23	2.13	0.48
2:B:50:ILE:HG22	2:B:145:GLN:OE1	2.13	0.48
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.95	0.48
1:A:332:GLN:O	1:A:336:GLN:HB2	2.13	0.48
1:A:260:LEU:O	1:A:264:LEU:HD23	2.14	0.48
2:B:111:VAL:HA	2:B:214:LEU:HD12	1.96	0.47
1:A:238:LYS:HG2	1:A:239:TRP:N	2.29	0.47
1:A:362:THR:HG22	1:A:366:LYS:HD3	1.96	0.47
1:A:317:VAL:HG12	1:A:318:TYR:H	1.79	0.47
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.96	0.47
1:A:371:ALA:HA	1:A:374:LYS:HE3	1.95	0.47
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.47	0.47
2:B:326:ILE:O	2:B:341:ILE:HA	2.13	0.47
1:A:380:ILE:CD1	1:A:386:THR:HG22	2.43	0.47
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.50	0.47
1:A:122:GLU:CD	1:A:122:GLU:H	2.18	0.47
2:B:332:GLN:OE1	2:B:424:LYS:HG2	2.15	0.47
1:A:116:PHE:HE1	1:A:146:TYR:CE2	2.33	0.47
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.55	0.47
1:A:237:ASP:OD2	1:A:238:LYS:HD2	2.15	0.46
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.74	0.46
1:A:317:VAL:HG12	1:A:318:TYR:N	2.29	0.46
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.97	0.46
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:H	2:B:66:LYS:HD2	1.81	0.46
1:A:184:MET:HB3	1:A:185:ASP:H	1.55	0.46
1:A:5:ILE:HD11	1:A:166:LYS:HD2	1.98	0.46
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.50	0.46
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.51	0.46
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.48	0.46
2:B:421:PRO:O	2:B:425:LEU:HD22	2.16	0.46
1:A:116:PHE:HE1	1:A:146:TYR:HE2	1.62	0.46
1:A:496:VAL:HA	1:A:534:ALA:O	2.16	0.46
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.43	0.46
1:A:249:LYS:O	1:A:252:TRP:NE1	2.49	0.46
1:A:498:ASP:HA	1:A:536:VAL:O	2.16	0.46
1:A:66:LYS:O	1:A:68:SER:HB2	2.16	0.46
1:A:279:LEU:HD23	1:A:302:GLU:OE2	2.15	0.46
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.15	0.45
1:A:98:ALA:HB1	1:A:383:TRP:CZ2	2.45	0.45
2:B:31:ILE:O	2:B:35:VAL:HG23	2.16	0.45
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.31	0.45
2:B:195:ILE:HG23	2:B:196:GLY:N	2.31	0.45
2:B:344:GLU:HB2	2:B:347:LYS:HD2	1.99	0.45
2:B:73:LYS:HB3	2:B:73:LYS:NZ	2.32	0.45
1:A:475:GLN:HG3	1:A:476:LYS:N	2.32	0.45
1:A:260:LEU:HD23	1:A:279:LEU:HD11	1.99	0.45
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.82	0.45
1:A:182:GLN:HG2	1:A:187:LEU:HD21	1.98	0.45
1:A:253:THR:HA	1:A:291:GLU:O	2.17	0.45
2:B:169:GLU:HG3	2:B:173:LYS:HE3	1.99	0.45
2:B:279:LEU:HA	2:B:282:LEU:HD12	1.99	0.45
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.52	0.45
1:A:224:GLU:O	3:A:999:SPP:HE2	2.16	0.44
3:A:999:SPP:C4	3:A:999:SPP:HB2	2.48	0.44
2:B:167:ILE:HD11	2:B:209:LEU:HD12	1.99	0.44
2:B:366:LYS:O	2:B:370:GLU:HG3	2.17	0.44
1:A:518:VAL:O	1:A:522:ILE:HG13	2.18	0.44
1:A:239:TRP:HZ2	1:A:349:LEU:O	2.01	0.44
2:B:379:SER:OG	2:B:387:PRO:HD3	2.18	0.44
2:B:254:VAL:HG21	2:B:287:LYS:HG3	1.99	0.44
1:A:246:LEU:HD22	1:A:260:LEU:HD11	2.00	0.44
2:B:122:GLU:HG3	2:B:123:ASP:N	2.33	0.44
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.63	0.44
1:A:20:LYS:HG3	1:A:55:PRO:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TRP:HZ3	2:B:403:THR:HG21	1.83	0.44
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.85	0.44
2:B:195:ILE:HG23	2:B:196:GLY:H	1.83	0.43
2:B:167:ILE:O	2:B:208:HIS:CE1	2.72	0.43
1:A:88:TRP:CZ3	2:B:57:ASN:HB2	2.53	0.43
1:A:100:LEU:HD11	3:A:999:SPP:HB1	2.00	0.43
1:A:238:LYS:HE3	1:A:240:THR:HG23	2.01	0.43
1:A:454:LYS:HA	1:A:467:VAL:O	2.17	0.43
1:A:503:LEU:HA	1:A:506:ILE:HD12	2.01	0.43
2:B:164:MET:HG2	2:B:182:GLN:NE2	2.34	0.43
2:B:303:LEU:O	2:B:307:ARG:HG3	2.19	0.43
1:A:521:ILE:O	1:A:525:LEU:HG	2.19	0.43
2:B:103:LYS:HE2	2:B:179:VAL:HG23	2.00	0.43
2:B:267:ALA:HB2	2:B:426:TRP:HE1	1.82	0.43
1:A:110:ASP:O	1:A:217:PRO:HD3	2.18	0.43
1:A:317:VAL:HG21	1:A:347:LYS:HG2	2.01	0.43
1:A:59:PRO:HG2	1:A:76:ASP:HB3	2.00	0.42
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.54	0.42
1:A:8:VAL:O	1:A:121:ASP:HB2	2.18	0.42
2:B:266:TRP:HZ3	2:B:426:TRP:CD2	2.38	0.42
1:A:91:GLN:NE2	2:B:137:ASN:O	2.52	0.42
2:B:210:LEU:C	2:B:212:TRP:H	2.23	0.42
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.82	0.42
3:A:999:SPP:H4	3:A:999:SPP:HC3	2.00	0.42
1:A:104:LYS:HE3	1:A:104:LYS:HB2	1.87	0.42
1:A:216:THR:CB	1:A:217:PRO:CD	2.88	0.42
1:A:236:PRO:HB3	3:A:999:SPP:C19	2.50	0.42
1:A:489:SER:HB2	1:A:493:VAL:HG22	2.01	0.42
2:B:107:THR:O	2:B:188:TYR:HA	2.19	0.42
1:A:244:ILE:O	1:A:244:ILE:HG23	2.21	0.41
1:A:475:GLN:HB2	1:A:475:GLN:HE21	1.60	0.41
1:A:499:SER:C	1:A:501:TYR:H	2.23	0.41
1:A:326:ILE:O	1:A:341:ILE:HA	2.19	0.41
2:B:254:VAL:O	2:B:258:GLN:HG3	2.21	0.41
2:B:43:LYS:HA	2:B:43:LYS:HD3	1.86	0.41
1:A:278:GLN:HG3	1:A:298:GLU:HB3	2.03	0.41
1:A:452:LEU:HD13	1:A:469:LEU:O	2.19	0.41
2:B:201:LYS:O	2:B:204:GLU:HB3	2.21	0.41
2:B:65:LYS:HB2	2:B:66:LYS:H	1.66	0.41
2:B:66:LYS:O	2:B:67:ASP:CB	2.69	0.41
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:O	1:A:261:VAL:HG23	2.19	0.41
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.51	0.41
1:A:357:MET:O	1:A:359:GLY:N	2.53	0.41
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.55	0.41
2:B:353:LYS:HB2	2:B:353:LYS:HE3	1.86	0.41
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.01	0.41
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.56	0.41
2:B:175:ASN:HB3	2:B:178:ILE:HD12	2.03	0.41
1:A:436:GLY:O	1:A:461:ARG:NH2	2.53	0.41
2:B:319:TYR:CZ	2:B:321:PRO:HA	2.56	0.41
1:A:255:ASN:OD1	1:A:289:LEU:HB3	2.19	0.41
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.56	0.41
1:A:431:LYS:HE3	1:A:431:LYS:HA	2.03	0.40
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.81	0.40
1:A:235:HIS:HB2	1:A:238:LYS:O	2.21	0.40
1:A:100:LEU:HD21	3:A:999:SPP:HB1	2.02	0.40
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.21	0.40
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.90	0.40
2:B:37:ILE:HD11	2:B:71:TRP:O	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	535/560 (96%)	482 (90%)	44 (8%)	9 (2%)	9	13
2	B	399/440 (91%)	376 (94%)	20 (5%)	3 (1%)	19	29
All	All	934/1000 (93%)	858 (92%)	64 (7%)	12 (1%)	12	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
2	B	195	ILE
1	A	230	MET
1	A	358	ARG
2	B	70	LYS
1	A	412	PRO
2	B	213	GLY
1	A	66	LYS
1	A	225	PRO
1	A	14	PRO
1	A	224	GLU
1	A	345	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	482/499 (97%)	431 (89%)	51 (11%)	6	10
2	B	369/400 (92%)	345 (94%)	24 (6%)	17	26
All	All	851/899 (95%)	776 (91%)	75 (9%)	10	14

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	20	LYS
1	A	64	LYS
1	A	65	LYS
1	A	69	THR
1	A	92	LEU
1	A	94	ILE
1	A	109	LEU
1	A	113	ASP
1	A	120	LEU
1	A	123	ASP
1	A	126	LYS

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Mol	Chain	Res	Type
1	A	139	THR
1	A	175	ASN
1	A	182	GLN
1	A	184	MET
1	A	197	GLN
1	A	205	LEU
1	A	210	LEU
1	A	215	THR
1	A	238	LYS
1	A	240	THR
1	A	242	GLN
1	A	243	PRO
1	A	250	ASP
1	A	283	LEU
1	A	332	GLN
1	A	340	GLN
1	A	347	LYS
1	A	353	LYS
1	A	356	ARG
1	A	357	MET
1	A	358	ARG
1	A	362	THR
1	A	368	LEU
1	A	373	GLN
1	A	386	THR
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	413	GLU
1	A	431	LYS
1	A	448	ARG
1	A	452	LEU
1	A	475	GLN
1	A	487	GLN
1	A	491	LEU
1	A	500	GLN
1	A	515	SER
1	A	517	LEU
1	A	523	GLU
2	B	8	VAL
2	B	24	TRP
2	B	29	GLU

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Mol	Chain	Res	Type
2	B	40	GLU
2	B	65	LYS
2	B	66	LYS
2	B	68	SER
2	B	73	LYS
2	B	167	ILE
2	B	194	GLU
2	B	201	LYS
2	B	209	LEU
2	B	214	LEU
2	B	215	THR
2	B	232	TYR
2	B	233	GLU
2	B	283	LEU
2	B	284	ARG
2	B	303	LEU
2	B	338	THR
2	B	361	HIS
2	B	362	THR
2	B	368	LEU
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	174	GLN
1	A	182	GLN
1	A	221	HIS
1	A	255	ASN
1	A	336	GLN
1	A	475	GLN
1	A	500	GLN
1	A	520	GLN
1	A	524	GLN
2	B	57	ASN
2	B	161	GLN
2	B	182	GLN
2	B	235	HIS
2	B	330	GLN
2	B	332	GLN
2	B	334	GLN

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Mol	Chain	Res	Type
2	B	340	GLN
2	B	394	GLN
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	3,7,8	0.74	0	1,8,10	4.03	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	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	4.03	113.20	105.54

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 carbohydrates 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	SPP	A	999	-	32,35,35	0.87	0	45,51,51	1.09	5 (11%)

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	SPP	A	999	-	-	4/18/31/31	0/4/4/4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	SPP	C18-C19-C20	-2.84	117.27	120.84
3	A	999	SPP	C14-N13-C20	2.46	109.58	104.45
3	A	999	SPP	OS2-S-OS1	-2.35	115.47	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	SPP	C17-C16-C21	-2.05	117.28	120.29
3	A	999	SPP	C8-C9-N10	-2.01	106.14	110.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

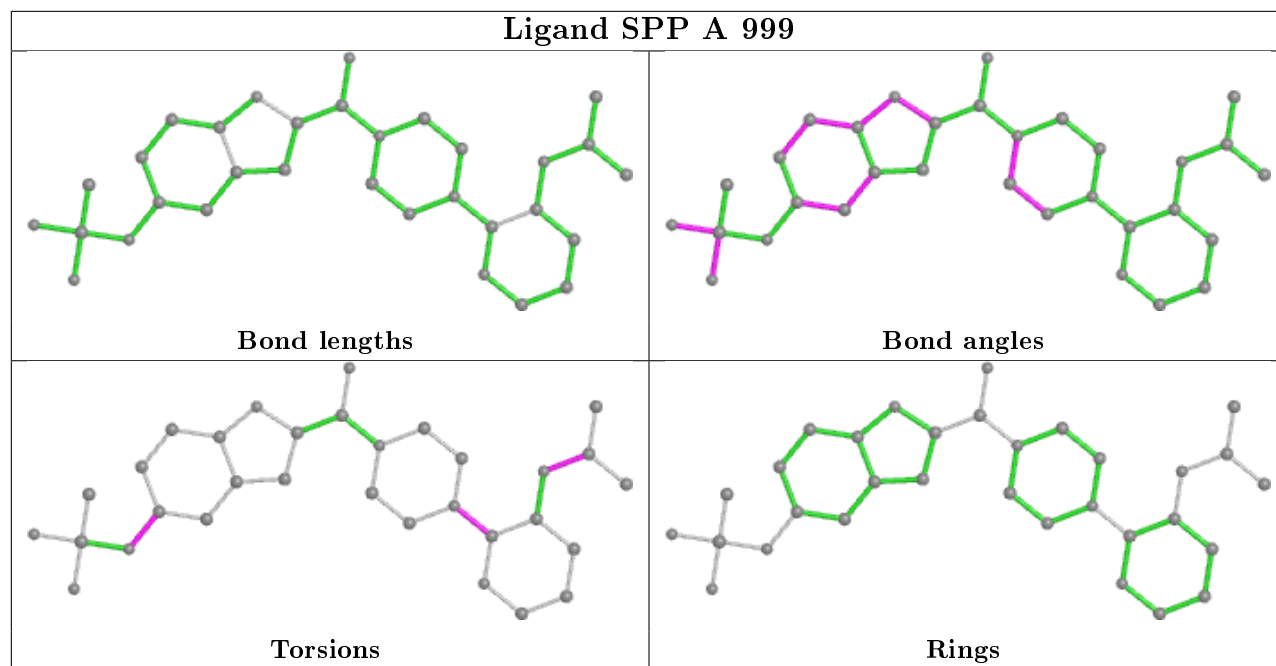
Mol	Chain	Res	Type	Atoms
3	A	999	SPP	CB-CA-N-C3
3	A	999	SPP	N1-C2-N7-C12
3	A	999	SPP	N1-C2-N7-C8
3	A	999	SPP	C18-C17-ND-S

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	SPP	10	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	537/560 (95%)	-0.05	27 (5%) 28 25	9, 44, 97, 144	0
2	B	405/440 (92%)	-0.23	11 (2%) 54 50	8, 39, 87, 112	0
All	All	942/1000 (94%)	-0.13	38 (4%) 38 34	8, 42, 92, 144	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	8.6
1	A	66	LYS	7.9
1	A	221	HIS	6.7
1	A	218	ASP	5.6
2	B	241	VAL	5.6
1	A	91	GLN	5.1
2	B	88	TRP	4.9
2	B	67	ASP	4.6
2	B	240	THR	4.6
1	A	220	LYS	4.5
2	B	213	GLY	4.4
2	B	232	TYR	4.3
1	A	219	LYS	4.1
1	A	52	PRO	3.9
1	A	137	ASN	3.8
1	A	356	ARG	3.6
1	A	223	LYS	3.4
2	B	214	LEU	3.4
1	A	69	THR	3.2
1	A	53	GLU	3.1
1	A	68	SER	3.1
2	B	433	PRO	2.9
1	A	22	LYS	2.8
1	A	24	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	224	GLU	2.6
1	A	136	ASN	2.5
1	A	539	HIS	2.5
1	A	358	ARG	2.4
1	A	2	ILE	2.3
1	A	346	PHE	2.3
1	A	135	ILE	2.3
2	B	6	GLU	2.2
1	A	70	LYS	2.1
1	A	51	GLY	2.1
2	B	174	GLN	2.1
2	B	66	LYS	2.0
1	A	225	PRO	2.0
1	A	446	ALA	2.0

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(\AA^2)	Q<0.9
1	CSD	A	280	8/9	0.96	0.11	27,31,38,41	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

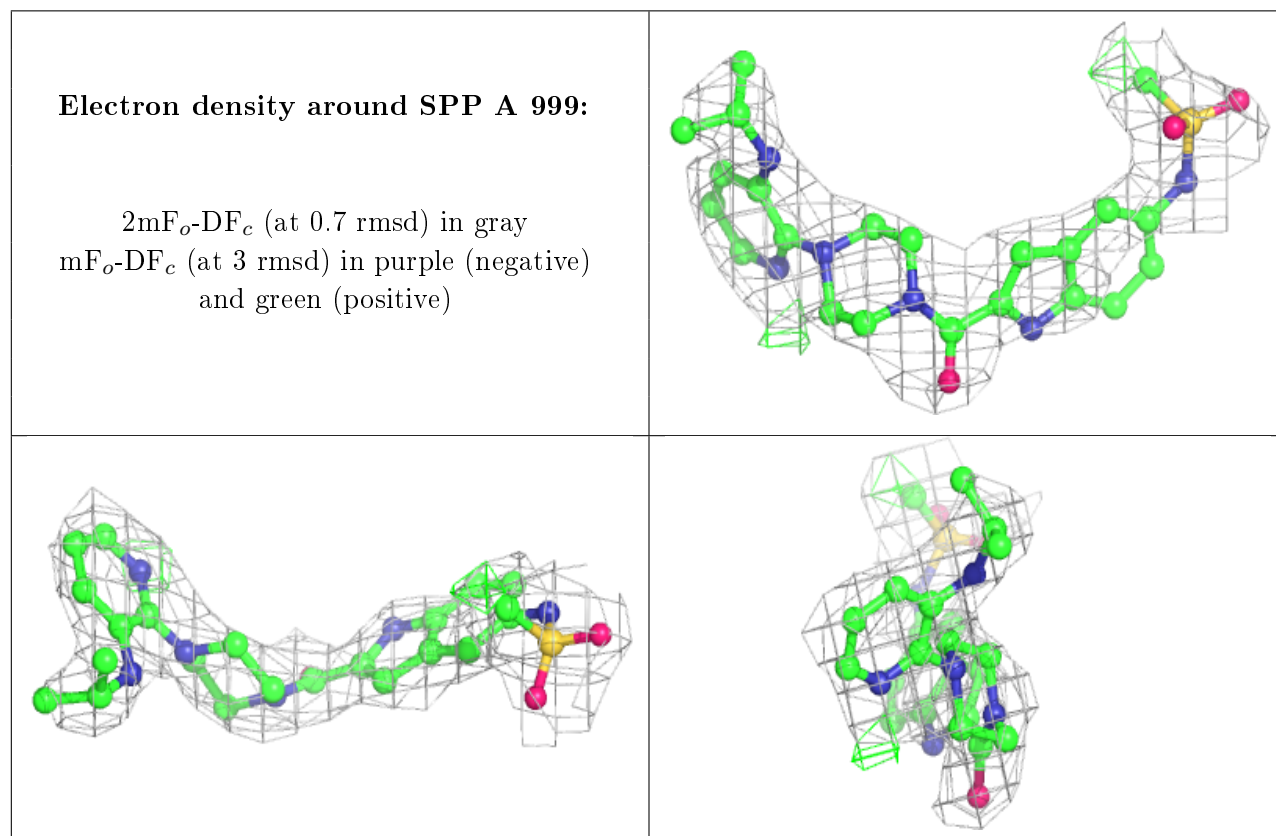
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	SPP	A	999	32/32	0.87	0.23	33,56,124,127	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 ⓘ

There are no such residues in this entry.