



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:03 PM UTC

PDB ID : 5J1E / pdb_00005j1e
Title : Crystal Structure of a Hydroxypyridone Carboxylic Acid Active-Site RNase H Inhibitor in Complex with HIV Reverse Transcriptase
Authors : Kirby, K.A.; Sarafianos, S.G.
Deposited on : 2016-03-29
Resolution : 2.90 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

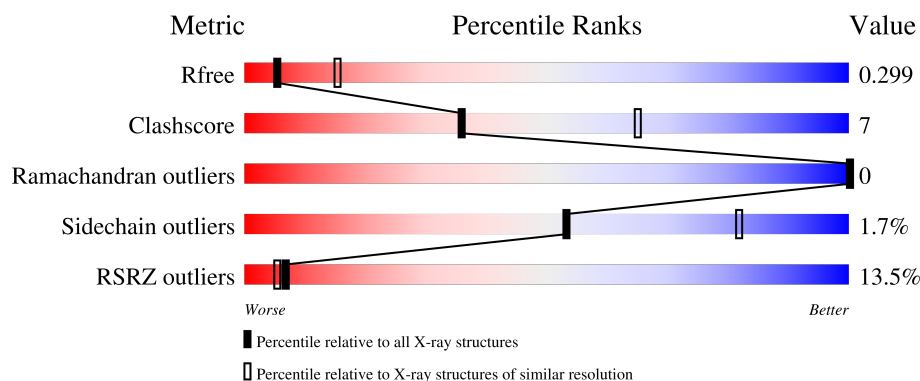
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	557	15% 71% 25% ..
1	C	557	11% 82% 16% ..
2	B	429	14% 75% 19% 6%
2	D	429	10% 73% 18% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15484 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 P66 DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4407	2855	730	815	7			
1	C	548	Total	C	N	O	S	0	0	0
			4463	2889	742	825	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
C	-1	MET	-	initiating methionine	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3341	2175	554	606	6			
2	D	393	Total	C	N	O	S	0	0	0
			3240	2114	532	589	5			

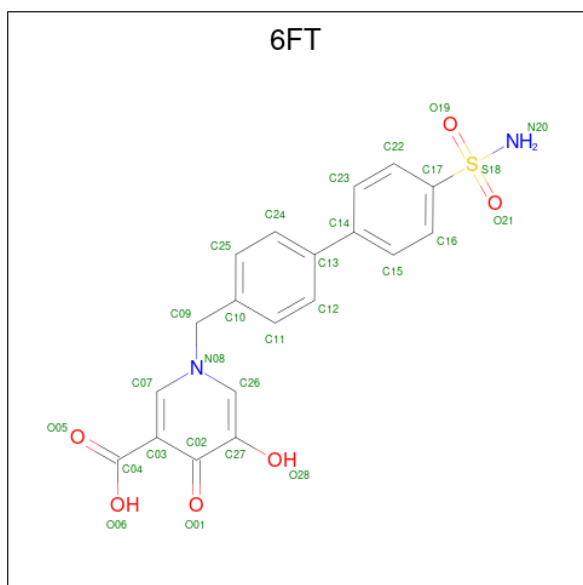
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is 5-hydroxy-4-oxo-1-[(4'-sulfamoyl[1,1'-biphenyl]-4-yl)methyl]-1,4-dihydropyridine-3-carboxylic acid (CCD ID: 6FT) (formula: C₁₉H₁₆N₂O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			28	19	2	6	1		

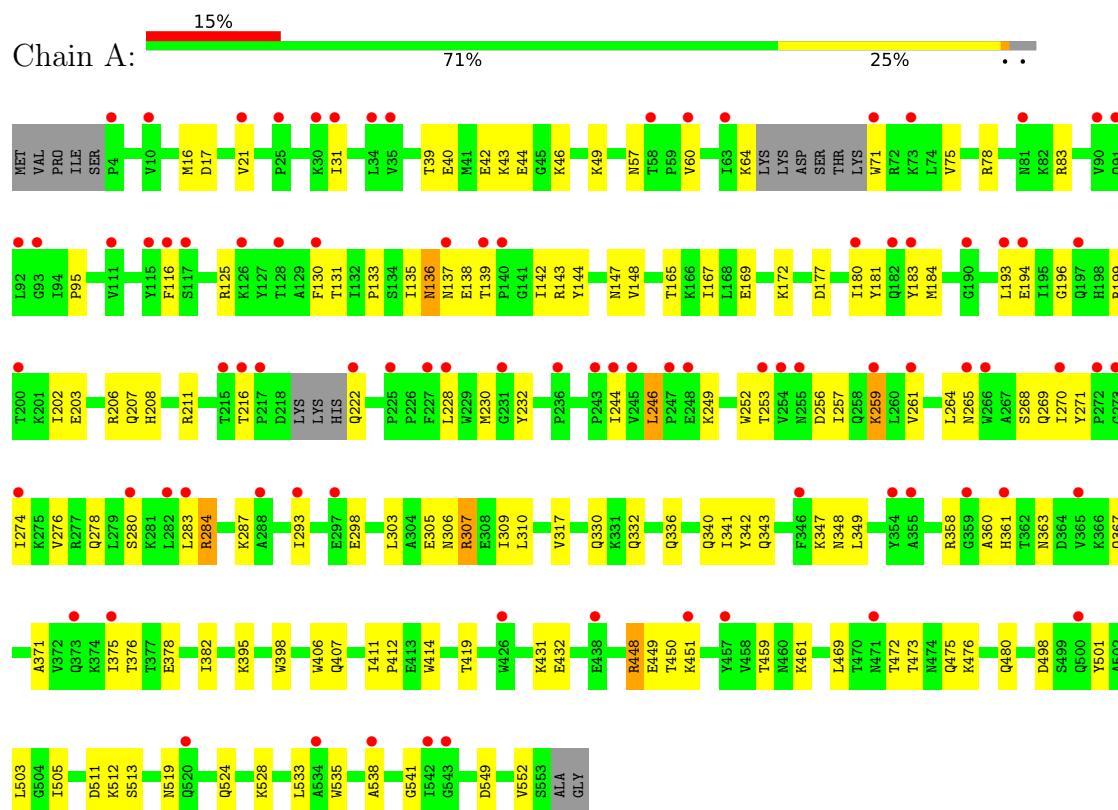
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0

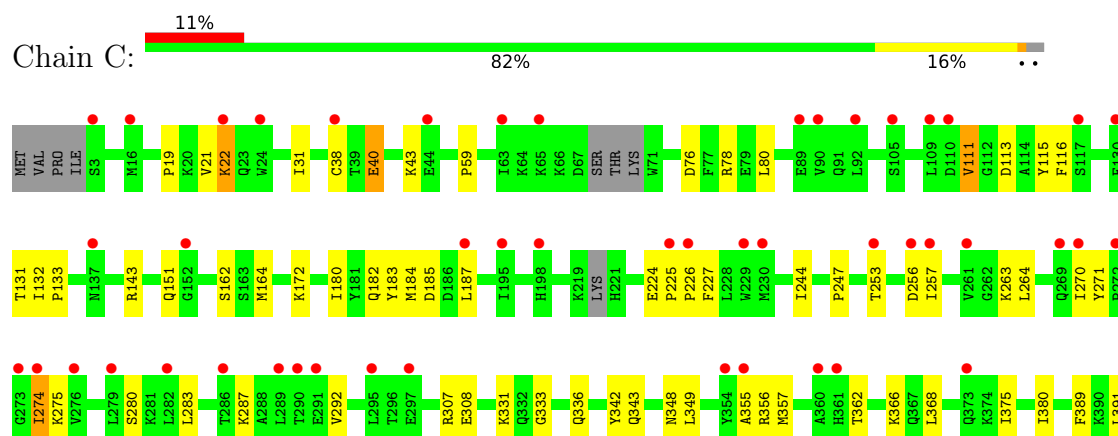
3 Residue-property plots [i](#)

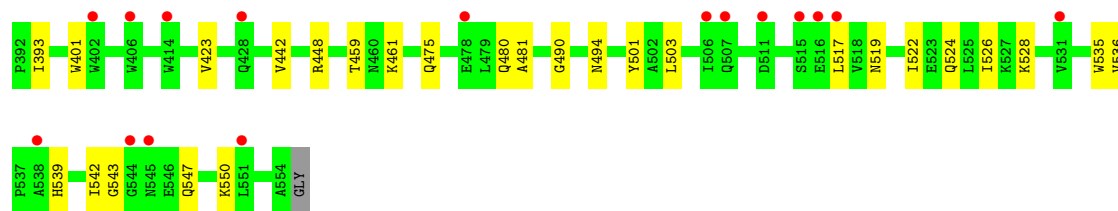
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 P66 DOMAIN

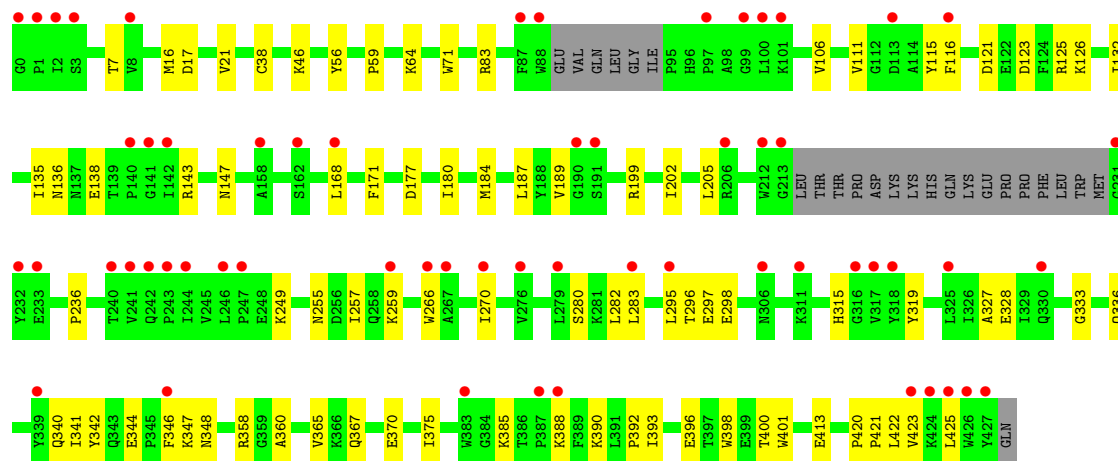


• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 DOMAIN

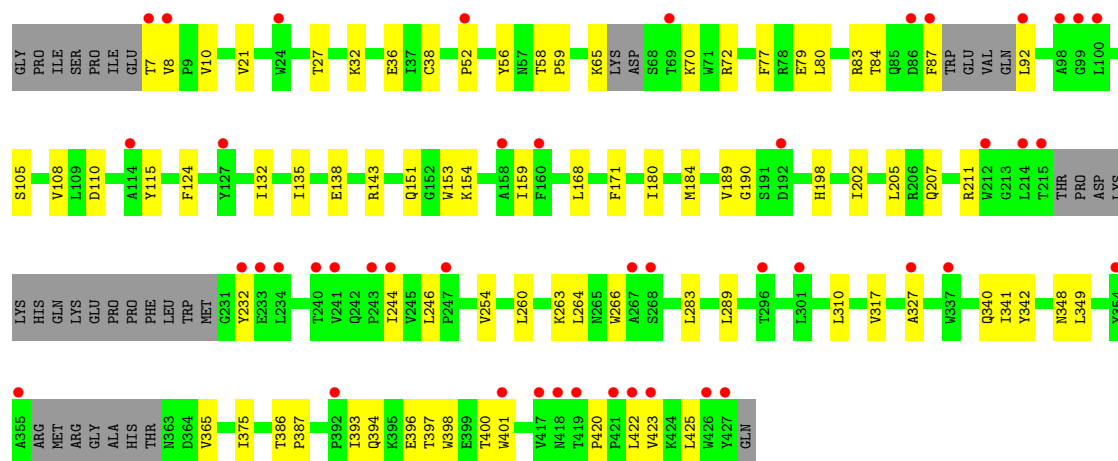




● Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 DOMAIN



● Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 DOMAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.07Å 89.31Å 108.22Å 105.47° 92.69° 110.80°	Depositor
Resolution (Å)	63.77 – 2.90 63.77 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (63.77-2.90) 97.8 (63.77-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.254 , 0.294 0.259 , 0.299	Depositor DCC
R_{free} test set	2495 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15484	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: MG, 6FT

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	0.13	0/4521	0.38	4/6143 (0.1%)
1	C	0.12	0/4578	0.33	0/6218
2	B	0.11	0/3437	0.30	0/4668
2	D	0.11	0/3329	0.29	0/4520
All	All	0.12	0/15865	0.33	4/21549 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASN	N-CA-C	7.41	121.29	108.76
1	A	419	THR	CA-C-N	6.12	124.13	119.66
1	A	419	THR	C-N-CA	6.12	124.13	119.66
1	A	137	ASN	N-CA-C	-6.08	97.84	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ASN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4407	0	4450	92	1
1	C	4463	0	4509	54	1
2	B	3341	0	3373	48	0
2	D	3240	0	3276	44	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
4	C	28	0	0	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
All	All	15484	0	15608	226	1

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 7.

All (226) 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:D:84:THR:HG21	2:D:153:TRP:HE1	1.42	0.84
1:C:59:PRO:HG2	1:C:76:ASP:HB3	1.61	0.82
1:A:83:ARG:NH2	1:C:308:GLU:OE1	2.16	0.79
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.67	0.76
1:A:246:LEU:HD21	1:A:310:LEU:HD12	1.69	0.73
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.71	0.72
1:C:459:THR:HG22	1:C:461:LYS:H	1.54	0.70
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.72	0.69
1:A:358:ARG:HG2	1:A:360:ALA:H	1.57	0.68
1:A:135:ILE:O	1:A:139:THR:OG1	2.11	0.68
1:A:83:ARG:HH22	1:C:308:GLU:CD	2.03	0.67
1:A:206:ARG:NH1	1:A:216:THR:O	2.27	0.65
1:A:459:THR:HG22	1:A:461:LYS:H	1.62	0.64
2:D:180:ILE:HG12	2:D:189:VAL:HG12	1.79	0.64
1:A:167:ILE:O	1:A:208:HIS:NE2	2.25	0.64
1:C:21:VAL:HB	1:C:59:PRO:HD3	1.81	0.63
1:C:224:GLU:HG2	1:C:226:PRO:HD2	1.80	0.63
2:B:135:ILE:O	2:B:138:GLU:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.81	0.62
1:A:228:LEU:HA	1:A:232:TYR:O	2.00	0.62
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.81	0.61
1:C:247:PRO:O	1:C:307:ARG:NH2	2.34	0.61
2:D:422:LEU:HG	2:D:425:LEU:HD12	1.83	0.60
1:A:472:THR:HA	1:A:476:LYS:HD2	1.82	0.60
2:B:168:LEU:HD22	2:B:205:LEU:HD11	1.84	0.60
1:C:356:ARG:HD2	1:C:362:THR:HG21	1.85	0.59
2:D:56:TYR:O	2:D:143:ARG:NH2	2.35	0.59
1:A:341:ILE:O	1:A:349:LEU:N	2.36	0.59
2:D:72:ARG:NH2	2:D:151:GLN:OE1	2.35	0.59
1:A:284:ARG:HH11	1:A:284:ARG:HB3	1.68	0.58
2:B:266:TRP:CE2	2:B:425:LEU:HD13	2.38	0.58
2:B:115:TYR:OH	2:B:184:MET:O	2.19	0.58
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.86	0.58
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.85	0.58
1:A:64:LYS:HB2	1:A:71:TRP:HA	1.86	0.57
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.87	0.57
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.86	0.57
2:D:87:PHE:HB3	2:D:92:LEU:HB3	1.87	0.56
1:C:244:ILE:HG23	1:C:263:LYS:HE2	1.87	0.56
1:C:480:GLN:HG2	1:C:517:LEU:HD11	1.87	0.56
1:A:524:GLN:O	1:A:528:LYS:HG2	2.04	0.56
2:D:79:GLU:HG3	2:D:83:ARG:HE	1.71	0.56
2:D:394:GLN:HB3	2:D:397:THR:HG22	1.87	0.56
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.87	0.56
1:C:78:ARG:NH2	1:C:287:LYS:O	2.31	0.55
1:C:164:MET:HE3	1:C:187:LEU:HD21	1.89	0.55
2:B:125:ARG:HD3	2:B:147:ASN:HD22	1.71	0.54
2:D:168:LEU:HD22	2:D:205:LEU:HD11	1.88	0.54
2:D:254:VAL:HG13	2:D:283:LEU:HD22	1.89	0.54
1:C:368:LEU:HD11	1:C:391:LEU:HD22	1.90	0.54
1:A:303:LEU:O	1:A:307:ARG:HB3	2.08	0.54
1:A:181:TYR:CD1	2:B:138:GLU:HB3	2.43	0.54
1:A:261:VAL:O	1:A:265:ASN:ND2	2.41	0.53
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.43	0.53
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.91	0.53
1:C:31:ILE:HG12	1:C:133:PRO:HG2	1.90	0.53
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.44	0.53
1:A:268:SER:OG	1:A:269:GLN:OE1	2.24	0.52
1:A:78:ARG:NH2	1:A:287:LYS:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ILE:HG23	1:C:271:TYR:HD1	1.73	0.52
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.91	0.52
2:B:106:VAL:HG12	2:B:236:PRO:HD3	1.91	0.52
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.32	0.52
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.91	0.51
1:A:259:LYS:N	1:A:259:LYS:HD2	2.25	0.51
1:C:375:ILE:HD11	1:C:389:PHE:HE1	1.75	0.51
1:A:199:ARG:HA	1:A:202:ILE:HD12	1.91	0.51
2:B:327:ALA:HA	2:B:340:GLN:O	2.11	0.51
1:C:333:GLY:H	1:C:336:GLN:HB2	1.75	0.51
1:C:355:ALA:HB1	1:C:357:MET:HE3	1.92	0.50
1:A:244:ILE:HB	1:A:310:LEU:HD13	1.92	0.50
2:B:111:VAL:HG11	2:B:187:LEU:HD12	1.93	0.50
2:D:246:LEU:HD13	2:D:260:LEU:HD11	1.93	0.50
1:A:95:PRO:HB2	1:A:230:MET:HE1	1.93	0.49
2:B:328:GLU:HG2	2:B:390:LYS:HB2	1.94	0.49
2:B:315:HIS:O	2:B:347:LYS:NZ	2.39	0.49
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.94	0.49
1:A:431:LYS:HG3	1:A:432:GLU:HG2	1.94	0.49
2:B:121:ASP:O	2:B:125:ARG:HG3	2.12	0.49
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.94	0.49
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.95	0.49
1:C:393:ILE:HB	1:C:423:VAL:HB	1.94	0.49
1:A:203:GLU:O	1:A:207:GLN:HG2	2.12	0.49
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.95	0.49
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.94	0.49
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.48	0.49
2:B:297:GLU:H	2:B:297:GLU:CD	2.20	0.49
2:B:255:ASN:O	2:B:259:LYS:HG2	2.13	0.48
1:A:549:ASP:HA	1:A:552:VAL:HG22	1.95	0.48
1:A:270:ILE:HG23	1:A:271:TYR:HD1	1.77	0.48
2:B:358:ARG:HE	2:B:370:GLU:HB2	1.79	0.48
1:A:317:VAL:HG21	1:A:347:LYS:HG2	1.95	0.48
1:C:183:TYR:HD1	1:C:184:MET:HG2	1.78	0.48
2:D:84:THR:HG22	2:D:124:PHE:HZ	1.79	0.48
1:A:44:GLU:HB3	1:A:46:LYS:HE3	1.94	0.48
1:A:284:ARG:HB3	1:A:284:ARG:NH1	2.28	0.48
2:B:333:GLY:O	2:B:336:GLN:HG2	2.14	0.48
1:A:249:LYS:NZ	1:A:256:ASP:OD2	2.47	0.48
2:D:396:GLU:O	2:D:400:THR:OG1	2.20	0.48
1:A:280:SER:HA	1:A:283:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.95	0.48
2:D:135:ILE:O	2:D:138:GLU:HG3	2.14	0.48
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.47
1:C:115:TYR:HD2	1:C:151:GLN:HA	1.79	0.47
2:D:32:LYS:HE2	2:D:36:GLU:OE2	2.15	0.47
1:A:222:GLN:OE1	1:A:228:LEU:N	2.44	0.47
1:A:473:THR:H	1:A:476:LYS:HB3	1.79	0.47
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.97	0.47
1:C:524:GLN:O	1:C:528:LYS:HG2	2.16	0.46
1:A:39:THR:O	1:A:43:LYS:HG3	2.15	0.46
1:A:44:GLU:HB2	1:A:46:LYS:HG2	1.97	0.46
1:A:172:LYS:HD3	1:A:180:ILE:HB	1.97	0.46
2:D:266:TRP:CG	2:D:425:LEU:HD13	2.50	0.46
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.50	0.46
1:A:278:GLN:CD	1:A:298:GLU:HB3	2.40	0.46
1:C:536:VAL:HB	1:C:542:ILE:HD12	1.96	0.46
1:C:380:ILE:HD12	2:D:27:THR:HG22	1.98	0.46
2:D:154:LYS:HA	2:D:184:MET:HE1	1.98	0.46
2:D:327:ALA:HA	2:D:340:GLN:O	2.16	0.46
1:A:375:ILE:HA	1:A:378:GLU:HG2	1.98	0.46
1:A:40:GLU:HA	1:A:43:LYS:HD2	1.98	0.46
1:A:253:THR:HG23	1:A:256:ASP:H	1.80	0.46
1:C:131:THR:HG22	1:C:143:ARG:HD2	1.97	0.46
2:D:198:HIS:O	2:D:202:ILE:HG12	2.16	0.46
1:A:306:ASN:O	1:A:309:ILE:HG13	2.16	0.46
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.97	0.46
1:A:541:GLY:O	2:B:280:SER:HB2	2.17	0.45
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.98	0.45
2:D:105:SER:O	2:D:190:GLY:HA2	2.16	0.45
1:A:131:THR:HG22	1:A:143:ARG:NE	2.32	0.45
1:A:332:GLN:HB2	1:A:336:GLN:HB2	1.98	0.45
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.97	0.45
2:D:420:PRO:HG2	2:D:422:LEU:HB2	1.98	0.45
2:B:396:GLU:O	2:B:400:THR:OG1	2.18	0.45
2:D:115:TYR:OH	2:D:184:MET:O	2.32	0.45
1:C:356:ARG:CD	1:C:362:THR:HG21	2.45	0.45
1:A:177:ASP:HB2	1:A:193:LEU:HD21	1.97	0.45
1:A:371:ALA:O	1:A:375:ILE:HG22	2.17	0.45
1:C:519:ASN:HA	1:C:522:ILE:HD12	1.99	0.45
1:A:165:THR:O	1:A:169:GLU:HG2	2.17	0.45
1:A:42:GLU:OE1	1:A:49:LYS:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:GLN:O	2:D:211:ARG:HD3	2.17	0.44
2:D:342:TYR:HB3	2:D:348:ASN:HA	1.99	0.44
1:A:257:ILE:O	1:A:261:VAL:HG13	2.16	0.44
2:D:317:VAL:HG22	2:D:349:LEU:HD23	1.98	0.44
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.53	0.44
2:B:17:ASP:O	2:B:83:ARG:HD3	2.17	0.44
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.57	0.44
2:B:266:TRP:CE3	2:B:425:LEU:HD22	2.52	0.44
2:D:171:PHE:CG	2:D:205:LEU:HD13	2.53	0.44
1:A:207:GLN:O	1:A:211:ARG:HG3	2.17	0.44
2:B:199:ARG:O	2:B:202:ILE:HG13	2.18	0.44
1:C:22:LYS:H	1:C:22:LYS:HD2	1.82	0.44
1:C:543:GLY:O	1:C:547:GLN:HG2	2.18	0.44
1:A:412:PRO:O	1:A:414:TRP:HD1	2.00	0.44
2:B:56:TYR:O	2:B:143:ARG:NH2	2.50	0.43
1:C:494:ASN:HB3	2:D:289:LEU:HD12	2.00	0.43
1:C:539:HIS:HB2	4:C:603:6FT:C12	2.49	0.43
1:A:230:MET:HE3	1:A:232:TYR:HE2	1.84	0.43
1:C:264:LEU:HD22	1:C:274:ILE:HD11	1.99	0.43
1:A:305:GLU:O	1:A:309:ILE:HG23	2.19	0.43
2:B:46:LYS:HE2	2:B:116:PHE:HB3	2.00	0.43
1:C:113:ASP:HB3	1:C:116:PHE:HB2	2.00	0.43
2:D:393:ILE:HD13	2:D:398:TRP:HB2	2.00	0.43
1:C:40:GLU:HA	1:C:43:LYS:HD3	2.01	0.43
2:D:65:LYS:NZ	2:D:110:ASP:OD2	2.50	0.43
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.54	0.43
1:C:331:LYS:HE2	1:C:333:GLY:O	2.19	0.43
1:C:490:GLY:O	1:C:528:LYS:NZ	2.49	0.43
1:A:57:ASN:OD1	1:A:131:THR:HG23	2.19	0.43
1:A:513:SER:O	1:A:519:ASN:ND2	2.52	0.43
2:B:297:GLU:HG2	2:B:298:GLU:H	1.84	0.43
1:C:172:LYS:HD3	1:C:180:ILE:HB	2.00	0.43
2:D:341:ILE:HD11	2:D:375:ILE:HG23	2.01	0.43
1:A:17:ASP:O	1:A:83:ARG:HD3	2.19	0.42
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.54	0.42
1:A:450:THR:O	1:A:451:LYS:HG2	2.18	0.42
1:C:225:PRO:O	1:C:227:PHE:N	2.47	0.42
1:A:183:TYR:CE2	1:A:184:MET:HE3	2.55	0.42
1:A:448:ARG:H	1:A:448:ARG:HG3	1.37	0.42
1:C:366:LYS:HE3	1:C:401:TRP:HH2	1.83	0.42
1:C:19:PRO:HD3	1:C:80:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:CYS:SG	1:C:132:ILE:HD11	2.59	0.42
1:C:256:ASP:OD1	1:C:257:ILE:N	2.52	0.42
1:A:503:LEU:HD12	1:A:533:LEU:HG	2.02	0.42
2:B:388:LYS:HD3	2:B:413:GLU:HB2	2.00	0.42
1:C:115:TYR:CD2	1:C:151:GLN:HA	2.54	0.42
2:D:80:LEU:O	2:D:84:THR:HG23	2.19	0.42
1:A:475:GLN:HB2	1:A:501:TYR:CD2	2.54	0.42
1:C:280:SER:HA	1:C:283:LEU:HD13	2.02	0.42
2:D:38:CYS:SG	2:D:132:ILE:HD11	2.60	0.42
1:A:21:VAL:O	1:A:57:ASN:ND2	2.53	0.42
2:D:58:THR:HG21	2:D:77:PHE:CD1	2.54	0.42
1:A:407:GLN:HG2	2:B:392:PRO:C	2.45	0.42
1:A:412:PRO:HD3	2:B:401:TRP:CZ2	2.55	0.42
2:B:360:ALA:HA	2:B:367:GLN:CD	2.44	0.42
1:C:270:ILE:HG23	1:C:271:TYR:CD1	2.54	0.42
2:D:108:VAL:HB	2:D:232:TYR:HB3	2.02	0.41
1:A:367:GLN:HE22	1:A:512:LYS:HE3	1.85	0.41
2:D:263:LYS:HA	2:D:425:LEU:HD22	2.02	0.41
2:B:16:MET:HG2	1:C:292:VAL:HG11	2.01	0.41
2:D:8:VAL:HG21	2:D:159:ILE:HD13	2.02	0.41
1:C:342:TYR:HB3	1:C:348:ASN:HA	2.03	0.41
2:D:266:TRP:CD2	2:D:425:LEU:HD13	2.55	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.21	0.41
2:B:123:ASP:O	2:B:126:LYS:NZ	2.54	0.41
2:B:177:ASP:OD1	2:B:177:ASP:N	2.51	0.41
1:A:131:THR:HG22	1:A:143:ARG:HE	1.86	0.41
1:A:172:LYS:HG2	1:A:180:ILE:HD12	2.02	0.41
1:A:194:GLU:CD	1:A:196:GLY:H	2.28	0.41
1:A:284:ARG:H	1:A:284:ARG:HG2	1.70	0.41
1:C:111:VAL:HG12	1:C:185:ASP:O	2.21	0.41
2:D:386:THR:HA	2:D:387:PRO:HD3	1.94	0.41
1:A:361:HIS:CD2	1:A:505:ILE:HG23	2.56	0.41
2:B:282:LEU:HD21	2:B:296:THR:HG23	2.03	0.41
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.96	0.41
1:C:162:SER:HB2	2:D:52:PRO:HG3	2.03	0.41
1:C:253:THR:HG23	1:C:256:ASP:H	1.85	0.41
1:A:116:PHE:C	1:A:148:VAL:HG21	2.46	0.40
1:A:270:ILE:HG23	1:A:271:TYR:CD1	2.55	0.40
2:B:171:PHE:CG	2:B:205:LEU:HD13	2.57	0.40
2:B:282:LEU:HD11	2:B:295:LEU:HA	2.04	0.40
2:D:244:ILE:HB	2:D:310:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TRP:O	1:A:293:ILE:HG22	2.21	0.40
1:A:382:ILE:O	2:B:136:ASN:HB2	2.21	0.40
2:B:319:TYR:OH	2:B:385:LYS:NZ	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:NZ	1:C:448:ARG:O[1_655]	2.18	0.02

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	535/557 (96%)	516 (96%)	19 (4%)	0	100	100
1	C	542/557 (97%)	526 (97%)	16 (3%)	0	100	100
2	B	399/429 (93%)	389 (98%)	10 (2%)	0	100	100
2	D	383/429 (89%)	374 (98%)	9 (2%)	0	100	100
All	All	1859/1972 (94%)	1805 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	483/497 (97%)	471 (98%)	12 (2%)	42	74
1	C	489/497 (98%)	481 (98%)	8 (2%)	55	83
2	B	367/390 (94%)	362 (99%)	5 (1%)	59	85
2	D	357/390 (92%)	353 (99%)	4 (1%)	65	88
All	All	1696/1774 (96%)	1667 (98%)	29 (2%)	53	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	A	142	ILE
1	A	246	LEU
1	A	259	LYS
1	A	264	LEU
1	A	274	ILE
1	A	276	VAL
1	A	284	ARG
1	A	307	ARG
1	A	395	LYS
1	A	448	ARG
1	A	449	GLU
2	B	7	THR
2	B	249	LYS
2	B	344	GLU
2	B	422	LEU
2	B	423	VAL
1	C	22	LYS
1	C	40	GLU
1	C	111	VAL
1	C	182	GLN
1	C	274	ILE
1	C	275	LYS
1	C	526	ILE
1	C	550	LYS
2	D	7	THR
2	D	10	VAL
2	D	70	LYS
2	D	423	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	407	GLN
1	A	487	GLN
2	B	147	ASN
2	B	161	GLN
2	B	361	HIS
2	B	373	GLN
2	B	394	GLN
1	C	147	ASN
1	C	336	GLN
1	C	487	GLN
2	D	137	ASN
2	D	161	GLN
2	D	269	GLN
2	D	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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
4	6FT	C	603	3	30,30,30	3.41	8 (26%)	42,44,44	2.18	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
4	6FT	C	603	3	-	9/18/18/18	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	6FT	C26-C27	11.93	1.53	1.35
4	C	603	6FT	C26-N08	6.93	1.49	1.36
4	C	603	6FT	C07-N08	6.88	1.49	1.36
4	C	603	6FT	C07-C03	5.69	1.53	1.38
4	C	603	6FT	S18-N20	5.56	1.71	1.60
4	C	603	6FT	C17-S18	3.07	1.81	1.77
4	C	603	6FT	C03-C04	2.86	1.53	1.48
4	C	603	6FT	O28-C27	2.52	1.40	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	6FT	O21-S18-O19	-11.29	101.43	118.80
4	C	603	6FT	O21-S18-C17	3.68	111.51	107.35
4	C	603	6FT	O19-S18-C17	3.12	110.88	107.35
4	C	603	6FT	O21-S18-N20	2.91	111.54	107.35
4	C	603	6FT	O19-S18-N20	2.56	111.04	107.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	603	6FT	C02-C03-C04-O05
4	C	603	6FT	C02-C03-C04-O06
4	C	603	6FT	C24-C13-C14-C23
4	C	603	6FT	C12-C13-C14-C15
4	C	603	6FT	C24-C13-C14-C15
4	C	603	6FT	C12-C13-C14-C23

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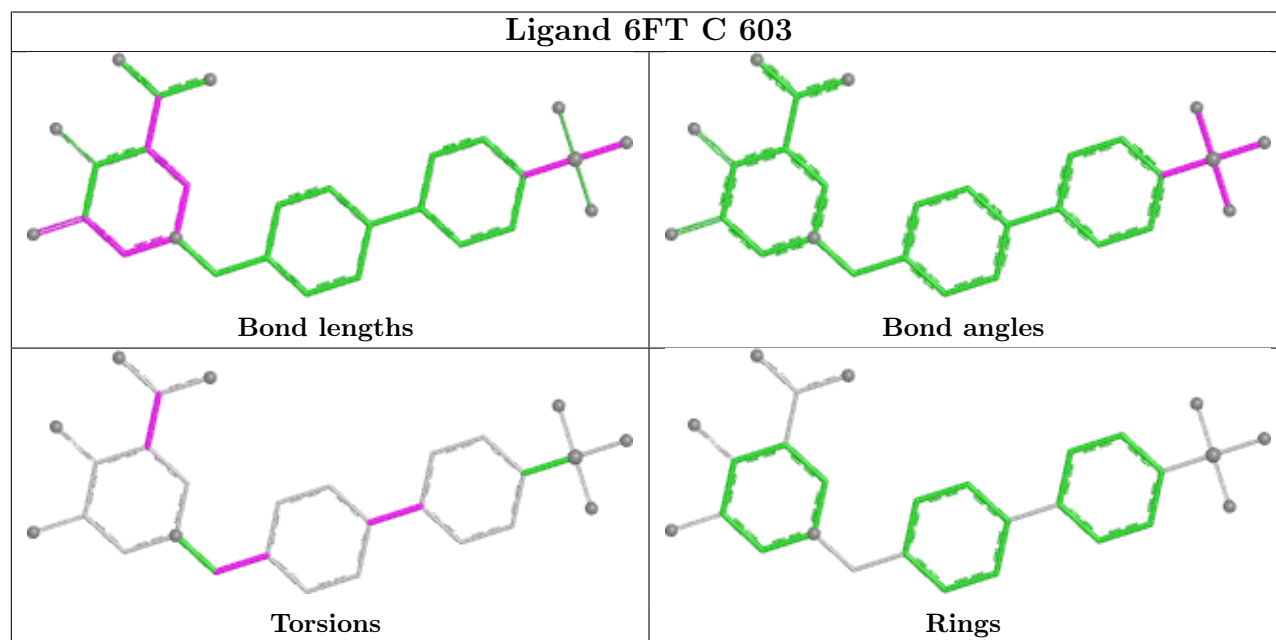
Mol	Chain	Res	Type	Atoms
4	C	603	6FT	C07-C03-C04-O06
4	C	603	6FT	C07-C03-C04-O05
4	C	603	6FT	N08-C09-C10-C11

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	6FT	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 ⓘ

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	541/557 (97%)	1.09	86 (15%) 5 4	36, 77, 138, 213	0
1	C	548/557 (98%)	0.99	64 (11%) 9 8	43, 70, 124, 166	0
2	B	405/429 (94%)	1.00	59 (14%) 6 4	36, 66, 124, 159	0
2	D	393/429 (91%)	0.95	45 (11%) 9 8	40, 60, 108, 126	0
All	All	1887/1972 (95%)	1.01	254 (13%) 7 5	36, 68, 126, 213	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	SER	5.9
2	D	114	ALA	5.3
1	C	272	PRO	4.7
2	D	423	VAL	4.5
2	B	426	TRP	4.4
2	D	422	LEU	4.4
1	C	282	LEU	4.3
2	D	232	TYR	4.3
1	C	297	GLU	4.3
2	B	279	LEU	4.1
1	A	500	GLN	4.1
2	D	267	ALA	4.1
2	D	233	GLU	4.1
2	D	421	PRO	4.0
2	B	231	GLY	3.9
1	A	183	TYR	3.9
1	C	551	LEU	3.9
2	B	88	TRP	3.8
1	A	236	PRO	3.8
1	A	34	LEU	3.8
1	A	31	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	93	GLY	3.7
2	B	283	LEU	3.5
1	A	216	THR	3.5
2	B	247	PRO	3.5
2	B	270	ILE	3.5
1	C	90	VAL	3.5
2	B	213	GLY	3.5
1	C	89	GLU	3.5
2	D	214	LEU	3.4
1	C	273	GLY	3.4
2	B	383	TRP	3.4
2	D	426	TRP	3.4
2	B	387	PRO	3.3
1	A	116	PHE	3.3
1	A	182	GLN	3.3
1	C	402	TRP	3.3
2	D	419	THR	3.3
1	A	255	ASN	3.3
2	B	325	LEU	3.3
1	C	515	SER	3.3
2	B	3	SER	3.3
2	D	327	ALA	3.3
2	B	295	LEU	3.2
1	A	139	THR	3.2
1	A	63	ILE	3.2
2	B	240	THR	3.2
2	B	140	PRO	3.2
2	B	212	TRP	3.2
2	B	232	TYR	3.1
2	D	427	TYR	3.1
2	D	99	GLY	3.1
1	A	361	HIS	3.1
2	B	242	GLN	3.1
2	D	87	PHE	3.1
2	D	268	SER	3.1
2	D	127	TYR	3.1
1	C	290	THR	3.1
2	D	86	ASP	3.0
1	A	270	ILE	3.0
2	D	92	LEU	3.0
1	C	531	VAL	3.0
2	D	160	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	101	LYS	3.0
2	D	243	PRO	3.0
1	C	92	LEU	3.0
1	A	21	VAL	3.0
2	B	142	ILE	3.0
2	B	316	GLY	3.0
1	C	256	ASP	3.0
2	B	346	PHE	3.0
1	A	293	ILE	2.9
1	A	35	VAL	2.9
1	A	254	VAL	2.9
2	B	266	TRP	2.9
1	C	261	VAL	2.9
2	D	7	THR	2.9
1	C	279	LEU	2.9
2	D	52	PRO	2.9
1	A	297	GLU	2.9
1	C	360	ALA	2.9
1	A	273	GLY	2.8
1	A	272	PRO	2.8
2	B	241	VAL	2.8
1	C	3	SER	2.8
1	C	506	ILE	2.8
1	A	90	VAL	2.8
2	D	98	ALA	2.8
2	D	158	ALA	2.8
1	A	280	SER	2.8
1	C	373	GLN	2.8
1	A	71	TRP	2.8
1	A	282	LEU	2.8
2	B	244	ILE	2.8
2	D	301	LEU	2.8
1	A	200	THR	2.8
2	D	296	THR	2.8
1	A	231	GLY	2.8
2	B	267	ALA	2.8
2	B	2	ILE	2.8
2	B	259	LYS	2.8
1	A	222	GLN	2.7
1	C	269	GLN	2.7
2	B	424	LYS	2.7
2	B	0	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	117	SER	2.7
2	B	317	VAL	2.7
1	A	73	LYS	2.7
2	B	311	LYS	2.7
1	A	10	VAL	2.7
1	A	542	ILE	2.7
1	C	295	LEU	2.7
1	A	359	GLY	2.7
1	A	197	GLN	2.7
2	D	241	VAL	2.7
1	C	289	LEU	2.7
2	D	100	LEU	2.7
1	A	266	TRP	2.6
1	A	58	THR	2.6
1	A	128	THR	2.6
1	A	91	GLN	2.6
2	D	8	VAL	2.6
1	A	217	PRO	2.6
1	A	137	ASN	2.6
2	B	246	LEU	2.6
1	A	225	PRO	2.6
2	B	243	PRO	2.6
1	A	180	ILE	2.6
2	B	233	GLU	2.6
1	A	140	PRO	2.5
1	C	544	GLY	2.5
1	C	253	THR	2.5
1	A	426	TRP	2.5
2	D	418	ASN	2.5
2	B	113	ASP	2.5
1	C	225	PRO	2.5
1	C	274	ILE	2.5
1	A	354	TYR	2.5
1	C	354	TYR	2.5
1	A	253	THR	2.5
1	A	259	LYS	2.5
1	A	265	ASN	2.5
1	A	283	LEU	2.5
1	C	226	PRO	2.5
1	C	406	TRP	2.5
2	D	212	TRP	2.5
1	C	478	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	2.4
2	D	244	ILE	2.4
1	C	152	GLY	2.4
1	A	438	GLU	2.4
2	B	318	TYR	2.4
2	B	330	GLN	2.4
2	B	388	LYS	2.4
1	A	81	ASN	2.4
1	A	190	GLY	2.4
2	D	417	VAL	2.4
2	B	191	SER	2.4
2	B	427	TYR	2.4
1	A	244	ILE	2.4
1	C	257	ILE	2.4
1	C	137	ASN	2.4
1	C	38	CYS	2.4
1	C	511	ASP	2.4
2	B	116	PHE	2.4
1	C	44	GLU	2.4
1	C	291	GLU	2.4
1	C	516	GLU	2.4
2	B	162	SER	2.4
1	C	24	TRP	2.4
1	A	228	LEU	2.4
1	C	361	HIS	2.4
2	B	276	VAL	2.3
2	B	423	VAL	2.3
1	A	543	GLY	2.3
1	A	538	ALA	2.3
1	C	198	HIS	2.3
1	C	63	ILE	2.3
1	C	286	THR	2.3
2	D	354	TYR	2.3
1	A	227	PHE	2.3
2	B	306	ASN	2.3
1	A	248	GLU	2.3
1	A	373	GLN	2.3
1	C	187	LEU	2.3
2	B	425	LEU	2.3
1	A	274	ILE	2.3
2	D	240	THR	2.3
1	A	243	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	230	MET	2.2
1	A	355	ALA	2.2
2	B	141	GLY	2.2
1	A	288	ALA	2.2
2	D	355	ALA	2.2
1	A	471	ASN	2.2
1	C	195	ILE	2.2
1	A	60	VAL	2.2
1	A	115	TYR	2.2
1	A	92	LEU	2.2
1	A	451	LYS	2.2
1	A	194	GLU	2.2
2	B	100	LEU	2.2
1	C	545	ASN	2.2
1	C	105	SER	2.2
1	C	109	LEU	2.2
1	A	534	ALA	2.2
1	C	538	ALA	2.2
1	A	261	VAL	2.2
2	D	192	ASP	2.2
2	D	215	THR	2.2
1	C	65	LYS	2.2
2	B	190	GLY	2.2
1	A	130	PHE	2.2
1	A	247	PRO	2.1
1	C	22	LYS	2.1
2	B	168	LEU	2.1
2	D	234	LEU	2.1
1	C	428	GLN	2.1
1	A	365	VAL	2.1
1	C	16	MET	2.1
1	C	517	LEU	2.1
2	B	158	ALA	2.1
1	A	111	VAL	2.1
1	A	4	PRO	2.1
2	B	1	PRO	2.1
2	D	24	TRP	2.1
2	D	337	TRP	2.1
1	A	457	TYR	2.1
2	B	339	TYR	2.1
1	A	520	GLN	2.1
1	C	507	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	247	PRO	2.1
2	D	392	PRO	2.1
1	C	130	PHE	2.1
2	B	87	PHE	2.1
1	C	110	ASP	2.1
2	B	206	ARG	2.1
1	C	270	ILE	2.1
1	C	355	ALA	2.1
1	A	126	LYS	2.0
2	B	8	VAL	2.0
2	B	97	PRO	2.0
2	B	99	GLY	2.0
1	A	375	ILE	2.0
1	C	229	TRP	2.0
2	D	401	TRP	2.0
1	C	276	VAL	2.0
1	A	25	PRO	2.0
1	A	346	PHE	2.0
1	A	215	THR	2.0
2	D	69	THR	2.0
1	A	30	LYS	2.0
1	C	414	TRP	2.0
1	A	245	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

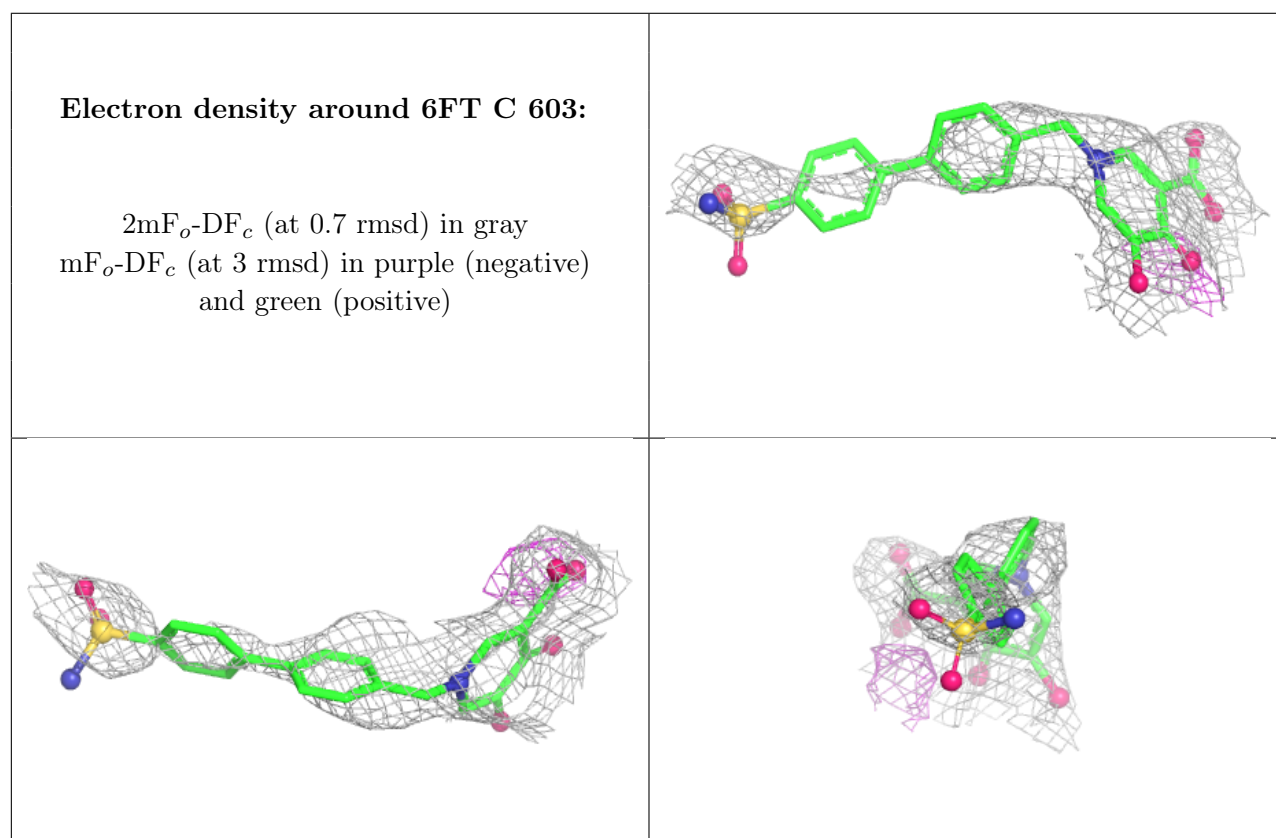
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	601	1/1	-0.13	0.29	113,113,113,113	0
4	6FT	C	603	28/28	0.68	0.21	60,82,99,101	28
3	MG	C	602	1/1	0.80	0.10	67,67,67,67	0
3	MG	C	601	1/1	0.89	0.14	66,66,66,66	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.