



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:56 AM UTC

PDB ID : 7KRF / pdb_00007krf
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with (E)-4-(3-(2-cyanovinyl)-5-fluorophenoxy)-3-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenyl sulfurofluoridate (JLJ710)
Authors : Bertoletti, N.; Ippolito, J.A.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2020-11-19
Resolution : 2.60 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

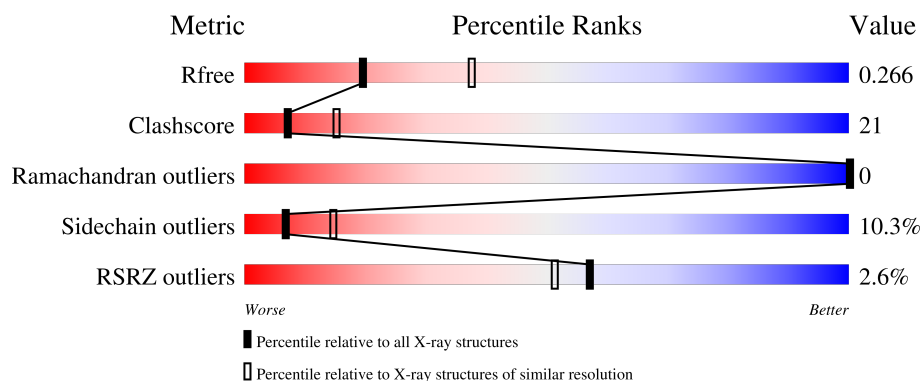
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	3% 57% 36% 5%
2	B	428	2% 60% 32% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7805 atoms, of which 15 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 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4416	2862	731	816	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

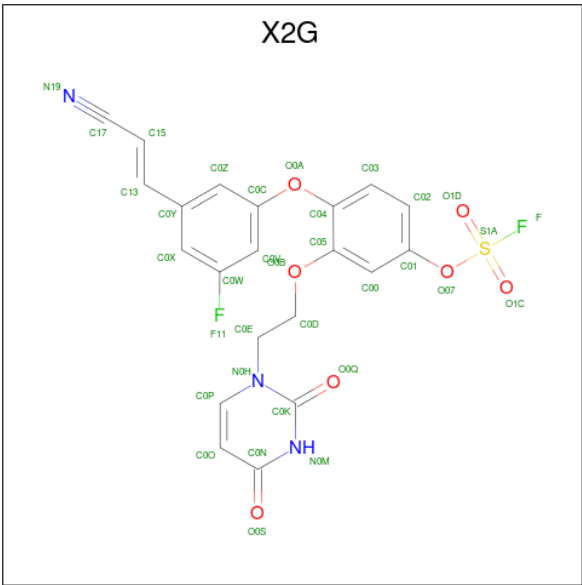
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE, P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	409	Total	C	N	O	S	0	0	0
			3341	2179	548	608	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-{3-[(E)-2-cyanoethenyl]-5-fluorophenoxy}-3-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenyl sulfurofluoridate (CCD ID: X2G) (formula: C₂₁H₁₅F₂N₃O₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	F	H	N	O	S		
3	A	1	48	21	1	15	3	7	1	0	0

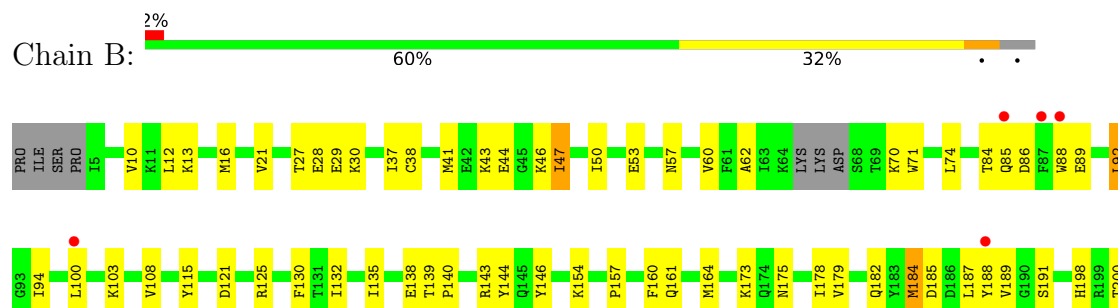
3 Residue-property plots

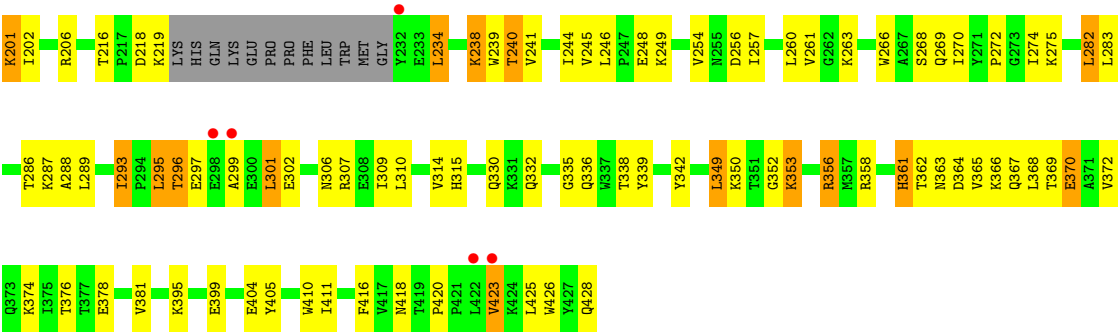
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE, P51 SUBUNIT





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.00Å 69.74Å 105.41Å 90.00° 105.59° 90.00°	Depositor
Resolution (Å)	57.79 – 2.60 57.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (57.79-2.60) 99.2 (57.79-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.221 , 0.265 0.232 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	97.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7805	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: X2G

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	0.12	0/4532	0.31	0/6169
2	B	0.08	0/3436	0.27	0/4676
All	All	0.11	0/7968	0.29	0/10845

There are no bond length outliers.

There are no bond angle outliers.

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	4416	0	4416	194	0
2	B	3341	0	3346	146	0
3	A	33	15	0	0	0
All	All	7790	15	7762	324	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 21.

All (324) 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:65:LYS:HA	1:A:72:ARG:HH11	1.08	1.13
1:A:454:LYS:HG3	1:A:552:VAL:HG13	1.46	0.96
2:B:342:TYR:HA	2:B:349:LEU:HD23	1.51	0.92
1:A:206:ARG:HH11	1:A:216:THR:HG23	1.36	0.90
1:A:65:LYS:HA	1:A:72:ARG:NH1	1.88	0.88
2:B:275:LYS:HB2	2:B:302:GLU:OE1	1.78	0.83
1:A:543:GLY:HA3	2:B:283:LEU:O	1.78	0.83
1:A:11:LYS:O	1:A:85:GLN:HG2	1.79	0.82
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.60	0.82
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.17	0.80
2:B:282:LEU:HD22	2:B:296:THR:HG23	1.64	0.79
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.48	0.79
1:A:252:TRP:HD1	1:A:295:LEU:HD11	1.47	0.78
1:A:295:LEU:N	1:A:295:LEU:HD13	1.95	0.78
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.63	0.78
2:B:245:VAL:O	2:B:263:LYS:NZ	2.17	0.78
2:B:270:ILE:O	2:B:272:PRO:HD3	1.84	0.78
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.64	0.77
2:B:295:LEU:H	2:B:295:LEU:HD12	1.49	0.77
1:A:295:LEU:H	1:A:295:LEU:HD22	1.49	0.76
1:A:88:TRP:CE2	2:B:143:ARG:HD2	2.19	0.76
2:B:206:ARG:NH1	2:B:216:THR:OG1	2.18	0.76
1:A:26:LEU:HD12	1:A:30:LYS:HD2	1.69	0.74
1:A:206:ARG:NH1	1:A:216:THR:HG23	2.03	0.73
2:B:238:LYS:NZ	2:B:238:LYS:HB3	2.03	0.73
1:A:134:SER:OG	1:A:139:THR:HG23	1.89	0.72
1:A:426:TRP:HB3	1:A:526:ILE:HD11	1.70	0.72
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.20	0.71
1:A:3:SER:HB2	1:A:5:ILE:HD12	1.72	0.70
2:B:282:LEU:HD22	2:B:296:THR:CG2	2.22	0.70
2:B:85:GLN:O	2:B:89:GLU:N	2.25	0.70
1:A:27:THR:O	1:A:31:ILE:HG13	1.92	0.69
1:A:30:LYS:HG2	1:A:71:TRP:CZ3	2.27	0.69
2:B:362:THR:HG22	2:B:366:LYS:NZ	2.07	0.69
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.20	0.69
2:B:358:ARG:CB	2:B:362:THR:HG23	2.22	0.69
2:B:254:VAL:HG23	2:B:283:LEU:CD2	2.23	0.68
2:B:244:ILE:HB	2:B:310:LEU:HD11	1.74	0.68
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.75	0.68
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.74	0.68
1:A:57:ASN:HD21	1:A:131:THR:HB	1.59	0.68
2:B:366:LYS:O	2:B:370:GLU:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:VAL:HA	2:B:88:TRP:HZ2	1.58	0.67
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.74	0.67
2:B:254:VAL:HG11	2:B:288:ALA:O	1.94	0.67
1:A:65:LYS:HB2	1:A:72:ARG:HD2	1.76	0.67
1:A:298:GLU:OE1	1:A:298:GLU:N	2.24	0.67
2:B:361:HIS:O	2:B:361:HIS:ND1	2.28	0.67
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.76	0.67
1:A:171:PHE:HB2	1:A:208:HIS:ND1	2.10	0.67
2:B:254:VAL:HG12	2:B:289:LEU:O	1.95	0.67
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.30	0.66
2:B:246:LEU:HD12	2:B:307:ARG:HG3	1.76	0.66
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.30	0.66
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.78	0.66
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.78	0.66
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.76	0.66
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.24	0.66
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.59	0.65
2:B:274:ILE:O	2:B:275:LYS:HE2	1.96	0.65
2:B:423:VAL:HG23	2:B:423:VAL:O	1.95	0.65
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.78	0.65
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.79	0.65
2:B:362:THR:HG22	2:B:366:LYS:HZ2	1.61	0.65
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.78	0.65
2:B:157:PRO:HG3	2:B:184:MET:HA	1.77	0.65
1:A:94:ILE:HG22	1:A:183:TYR:HE1	1.62	0.64
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.78	0.64
2:B:239:TRP:HB3	2:B:350:LYS:HE2	1.79	0.64
1:A:519:ASN:O	1:A:523:GLU:HG2	1.96	0.64
1:A:324:ASP:O	1:A:343:GLN:HG2	1.97	0.64
2:B:12:LEU:HD13	2:B:84:THR:HG22	1.79	0.63
1:A:116:PHE:HA	1:A:148:VAL:CG2	2.28	0.63
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.78	0.63
1:A:512:LYS:HZ2	1:A:512:LYS:HB3	1.63	0.63
1:A:23:GLN:HG2	1:A:131:THR:HG22	1.79	0.62
1:A:454:LYS:CG	1:A:552:VAL:HG13	2.28	0.61
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.30	0.61
1:A:255:ASN:HB2	1:A:289:LEU:HD21	1.82	0.61
1:A:137:ASN:O	1:A:137:ASN:ND2	2.27	0.61
2:B:30:LYS:HG2	2:B:62:ALA:HB3	1.83	0.61
1:A:503:LEU:HD12	1:A:533:LEU:HD23	1.81	0.61
1:A:296:THR:HG23	1:A:299:ALA:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:LYS:HE2	2:B:399:GLU:OE2	2.00	0.60
1:A:3:SER:HB3	1:A:4:PRO:HD2	1.83	0.60
2:B:257:ILE:O	2:B:261:VAL:HG23	2.01	0.60
1:A:57:ASN:HD22	1:A:143:ARG:HH12	1.50	0.60
1:A:282:LEU:HD21	1:A:296:THR:CG2	2.31	0.59
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.85	0.59
1:A:79:GLU:O	1:A:83:ARG:NH1	2.36	0.59
1:A:22:LYS:HD2	1:A:24:TRP:HE1	1.68	0.58
1:A:65:LYS:HD2	1:A:65:LYS:C	2.28	0.58
1:A:233:GLU:OE2	1:A:243:PRO:HD3	2.03	0.58
2:B:254:VAL:CG1	2:B:289:LEU:HA	2.33	0.58
1:A:57:ASN:HD22	1:A:143:ARG:NH1	2.01	0.58
2:B:362:THR:HB	2:B:366:LYS:HD3	1.84	0.58
1:A:537:PRO:HB2	1:A:540:LYS:HG3	1.85	0.58
1:A:65:LYS:CA	1:A:72:ARG:HH11	2.00	0.58
2:B:37:ILE:HD11	2:B:71:TRP:O	2.03	0.58
1:A:255:ASN:HB2	1:A:289:LEU:CD2	2.34	0.57
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.86	0.57
2:B:244:ILE:O	2:B:310:LEU:HD21	2.05	0.57
1:A:410:TRP:HZ3	2:B:405:TYR:HE1	1.51	0.57
2:B:10:VAL:HG13	2:B:88:TRP:CZ2	2.40	0.57
2:B:362:THR:CG2	2:B:366:LYS:HD3	2.35	0.57
1:A:171:PHE:HB2	1:A:208:HIS:CE1	2.39	0.57
1:A:194:GLU:OE1	1:A:194:GLU:HA	2.06	0.56
1:A:406:TRP:CE2	2:B:420:PRO:HB3	2.40	0.56
1:A:21:VAL:HG12	1:A:22:LYS:N	2.20	0.56
2:B:198:HIS:O	2:B:202:ILE:HG12	2.06	0.56
1:A:22:LYS:HD2	1:A:24:TRP:NE1	2.21	0.56
1:A:441:TYR:O	1:A:548:VAL:HG11	2.05	0.56
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.88	0.55
1:A:317:VAL:HG11	1:A:347:LYS:CD	2.37	0.55
2:B:254:VAL:HG23	2:B:283:LEU:HD23	1.89	0.55
1:A:334:GLN:H	1:A:334:GLN:HE21	1.54	0.55
1:A:317:VAL:HG23	1:A:349:LEU:HD13	1.89	0.55
1:A:30:LYS:HG2	1:A:71:TRP:CH2	2.40	0.55
2:B:37:ILE:O	2:B:41:MET:HG3	2.07	0.54
1:A:91:GLN:HE22	1:A:183:TYR:HA	1.71	0.54
1:A:130:PHE:CE2	1:A:144:TYR:HB3	2.42	0.54
2:B:266:TRP:O	2:B:269:GLN:HG3	2.07	0.54
2:B:44:GLU:OE1	2:B:46:LYS:NZ	2.40	0.54
2:B:240:THR:OG1	2:B:241:VAL:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HD21	2:B:295:LEU:HA	1.89	0.54
1:A:406:TRP:CD1	2:B:420:PRO:HB3	2.42	0.54
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.43	0.54
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.38	0.54
2:B:423:VAL:HB	2:B:426:TRP:HE3	1.72	0.53
1:A:191:SER:OG	1:A:198:HIS:ND1	2.41	0.53
2:B:53:GLU:OE1	2:B:53:GLU:N	2.41	0.53
1:A:235:HIS:HB2	1:A:238:LYS:HG2	1.90	0.53
2:B:100:LEU:HG	2:B:381:VAL:HG13	1.89	0.53
1:A:295:LEU:N	1:A:295:LEU:CD1	2.66	0.53
1:A:202:ILE:O	1:A:206:ARG:HG3	2.08	0.53
1:A:94:ILE:HG22	1:A:183:TYR:CE1	2.42	0.53
1:A:296:THR:HG23	1:A:299:ALA:CB	2.39	0.53
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.91	0.53
2:B:314:VAL:HG12	2:B:315:HIS:N	2.24	0.52
1:A:426:TRP:HB3	1:A:526:ILE:CD1	2.38	0.52
2:B:363:ASN:O	2:B:367:GLN:HG3	2.09	0.52
1:A:210:LEU:O	1:A:210:LEU:HD12	2.10	0.52
1:A:271:TYR:CE2	1:A:314:VAL:HG12	2.44	0.52
2:B:175:ASN:OD1	2:B:201:LYS:HE3	2.09	0.52
1:A:443:ASP:OD2	1:A:444:GLY:N	2.42	0.52
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.39	0.52
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.44	0.52
1:A:64:LYS:H	1:A:64:LYS:HD2	1.74	0.52
1:A:282:LEU:HD21	1:A:296:THR:HG22	1.90	0.52
1:A:427:TYR:CE1	1:A:525:LEU:HD13	2.45	0.51
1:A:57:ASN:ND2	1:A:131:THR:HB	2.24	0.51
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.93	0.51
1:A:544:GLY:HA2	2:B:286:THR:CG2	2.39	0.51
1:A:473:THR:O	1:A:477:THR:HG23	2.10	0.51
2:B:254:VAL:HG23	2:B:283:LEU:HD22	1.92	0.51
1:A:291:GLU:HG3	1:A:291:GLU:O	2.11	0.51
1:A:324:ASP:OD2	1:A:388:LYS:NZ	2.44	0.51
2:B:10:VAL:HA	2:B:88:TRP:CZ2	2.44	0.51
1:A:132:ILE:HG13	1:A:142:ILE:HB	1.93	0.50
2:B:295:LEU:HD12	2:B:295:LEU:N	2.23	0.50
2:B:362:THR:CB	2:B:366:LYS:HD3	2.41	0.50
1:A:65:LYS:HB2	1:A:72:ARG:CD	2.42	0.50
1:A:88:TRP:CD2	2:B:143:ARG:HD2	2.46	0.50
2:B:423:VAL:HB	2:B:426:TRP:CE3	2.46	0.50
1:A:290:THR:O	1:A:290:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.92	0.50
1:A:434:ILE:HD13	1:A:530:LYS:HB2	1.94	0.50
1:A:441:TYR:O	1:A:548:VAL:HG21	2.12	0.50
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.42	0.49
2:B:191:SER:OG	2:B:198:HIS:ND1	2.32	0.49
1:A:111:VAL:HG13	1:A:185:ASP:O	2.12	0.49
1:A:53:GLU:H	1:A:53:GLU:CD	2.17	0.49
2:B:254:VAL:CG2	2:B:283:LEU:HD22	2.43	0.49
1:A:252:TRP:O	1:A:292:VAL:HG13	2.12	0.49
1:A:252:TRP:CD1	1:A:295:LEU:CD1	2.92	0.49
1:A:279:LEU:HD12	1:A:302:GLU:OE1	2.13	0.49
1:A:410:TRP:HB2	2:B:365:VAL:HG21	1.95	0.49
1:A:420:PRO:HA	1:A:421:PRO:C	2.38	0.49
1:A:21:VAL:HG12	1:A:22:LYS:H	1.77	0.49
1:A:410:TRP:HD1	1:A:412:PRO:HD3	1.78	0.49
2:B:362:THR:HG22	2:B:366:LYS:HD3	1.94	0.48
2:B:301:LEU:HD23	2:B:302:GLU:HG2	1.95	0.48
1:A:384:GLY:O	2:B:27:THR:HG23	2.14	0.48
2:B:428:GLN:OE1	2:B:428:GLN:HA	2.13	0.48
1:A:491:LEU:HD13	1:A:529:GLU:OE2	2.13	0.48
1:A:512:LYS:HZ2	1:A:512:LYS:CB	2.25	0.48
1:A:406:TRP:NE1	2:B:420:PRO:HB3	2.28	0.48
2:B:249:LYS:HE3	2:B:256:ASP:OD1	2.13	0.48
1:A:50:ILE:CG1	1:A:143:ARG:HB3	2.44	0.48
2:B:27:THR:HG22	2:B:29:GLU:H	1.78	0.48
1:A:53:GLU:O	1:A:55:PRO:HD3	2.12	0.48
1:A:171:PHE:HE1	1:A:204:GLU:HG3	1.78	0.48
2:B:21:VAL:O	2:B:57:ASN:ND2	2.28	0.48
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.48	0.48
1:A:398:TRP:CH2	1:A:411:ILE:HG23	2.48	0.48
1:A:544:GLY:HA2	2:B:286:THR:CB	2.44	0.48
2:B:206:ARG:NH1	2:B:218:ASP:HB2	2.28	0.48
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.48	0.48
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.49	0.48
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.48	0.48
2:B:353:LYS:HE2	2:B:428:GLN:OE1	2.14	0.48
1:A:297:GLU:H	1:A:297:GLU:HG2	1.36	0.48
1:A:389:PHE:O	1:A:414:TRP:HA	2.13	0.47
1:A:195:ILE:HD13	1:A:195:ILE:N	2.29	0.47
1:A:326:ILE:HD12	1:A:326:ILE:N	2.30	0.47
2:B:206:ARG:NH2	2:B:219:LYS:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG13	1:A:161:GLN:NE2	2.29	0.47
1:A:447:ASN:OD1	1:A:450:THR:HG23	2.14	0.47
1:A:522:ILE:O	1:A:526:ILE:HG12	2.15	0.47
2:B:135:ILE:O	2:B:138:GLU:HG3	2.14	0.47
2:B:179:VAL:O	2:B:189:VAL:HA	2.14	0.47
2:B:246:LEU:HD22	2:B:260:LEU:CD1	2.44	0.47
2:B:12:LEU:CD1	2:B:84:THR:HG22	2.45	0.47
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.97	0.47
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.80	0.47
1:A:3:SER:C	1:A:5:ILE:H	2.23	0.47
2:B:13:LYS:HB3	2:B:16:MET:HG3	1.97	0.47
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.45	0.47
2:B:286:THR:O	2:B:286:THR:OG1	2.31	0.47
2:B:362:THR:HG22	2:B:366:LYS:CD	2.45	0.47
1:A:298:GLU:H	1:A:298:GLU:CD	2.19	0.46
1:A:317:VAL:HG11	1:A:347:LYS:HD2	1.96	0.46
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.80	0.46
2:B:309:ILE:HG12	2:B:309:ILE:O	2.15	0.46
2:B:361:HIS:O	2:B:361:HIS:CG	2.68	0.46
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.45	0.46
1:A:213:GLY:O	1:A:214:LEU:HD23	2.15	0.46
1:A:277:ARG:NH1	1:A:334:GLN:HG3	2.30	0.46
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.56	0.45
2:B:189:VAL:HG23	2:B:189:VAL:O	2.15	0.45
2:B:332:GLN:HB2	2:B:336:GLN:O	2.16	0.45
2:B:374:LYS:O	2:B:378:GLU:HG3	2.16	0.45
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.51	0.45
2:B:164:MET:HE3	2:B:182:GLN:NE2	2.32	0.45
2:B:274:ILE:C	2:B:275:LYS:HE2	2.42	0.45
2:B:282:LEU:O	2:B:282:LEU:HD12	2.16	0.45
2:B:368:LEU:O	2:B:372:VAL:HG23	2.16	0.45
2:B:257:ILE:CG2	2:B:283:LEU:HD11	2.46	0.45
1:A:39:THR:O	1:A:43:LYS:HG3	2.17	0.45
2:B:240:THR:O	2:B:350:LYS:HD2	2.17	0.45
2:B:296:THR:HG23	2:B:299:ALA:HB2	1.98	0.45
1:A:54:ASN:O	1:A:143:ARG:NH2	2.50	0.44
2:B:238:LYS:HB3	2:B:238:LYS:HZ3	1.80	0.44
1:A:218:ASP:O	1:A:219:LYS:C	2.61	0.44
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.53	0.44
1:A:410:TRP:HZ3	2:B:405:TYR:CE1	2.33	0.44
1:A:377:THR:O	1:A:381:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PRO:HD2	1:A:53:GLU:CD	2.42	0.44
1:A:516:GLU:HA	1:A:519:ASN:ND2	2.26	0.44
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.48	0.44
1:A:259:LYS:HB2	1:A:259:LYS:HE3	1.75	0.44
1:A:363:ASN:HB3	1:A:510:PRO:HA	2.00	0.44
1:A:148:VAL:HG23	1:A:149:LEU:N	2.33	0.43
2:B:115:TYR:HE1	2:B:185:ASP:OD1	2.00	0.43
1:A:3:SER:HB2	1:A:5:ILE:CD1	2.47	0.43
1:A:357:MET:HB3	1:A:358:ARG:H	1.64	0.43
2:B:139:THR:HB	2:B:140:PRO:HD2	1.98	0.43
1:A:116:PHE:HD2	1:A:148:VAL:HG21	1.82	0.43
1:A:542:ILE:HG22	1:A:543:GLY:N	2.32	0.43
2:B:370:GLU:HG2	2:B:370:GLU:H	1.66	0.43
1:A:73:LYS:HE2	1:A:75:VAL:HG23	2.00	0.43
1:A:144:TYR:O	1:A:145:GLN:HB3	2.17	0.43
1:A:130:PHE:CD2	1:A:130:PHE:N	2.85	0.43
1:A:164:MET:HE1	1:A:214:LEU:HD13	2.00	0.43
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.53	0.43
2:B:43:LYS:HE3	2:B:43:LYS:HB2	1.69	0.43
2:B:88:TRP:CZ3	2:B:92:LEU:HD22	2.53	0.43
1:A:540:LYS:HB2	1:A:542:ILE:HD12	2.00	0.43
1:A:73:LYS:HE2	1:A:75:VAL:CG2	2.49	0.43
1:A:113:ASP:O	1:A:114:ALA:C	2.61	0.43
1:A:532:TYR:CE1	1:A:534:ALA:HB2	2.54	0.43
2:B:356:ARG:HA	2:B:356:ARG:HD3	1.87	0.43
1:A:68:SER:OG	1:A:69:THR:N	2.50	0.43
1:A:102:LYS:HD2	1:A:103:LYS:N	2.34	0.43
1:A:219:LYS:HD2	1:A:220:LYS:H	1.83	0.42
2:B:274:ILE:HG23	2:B:306:ASN:ND2	2.34	0.42
2:B:369:THR:HG21	2:B:405:TYR:HB2	2.01	0.42
1:A:90:VAL:HG12	1:A:91:GLN:N	2.34	0.42
2:B:295:LEU:H	2:B:295:LEU:CD1	2.28	0.42
1:A:38:CYS:HB3	1:A:144:TYR:CZ	2.54	0.42
1:A:271:TYR:CD2	1:A:314:VAL:HG12	2.54	0.42
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.19	0.42
1:A:32:LYS:O	1:A:36:GLU:HG3	2.20	0.42
1:A:266:TRP:O	1:A:269:GLN:HG2	2.19	0.42
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.55	0.42
2:B:74:LEU:HD21	2:B:411:ILE:HD11	2.02	0.42
1:A:230:MET:HA	1:A:230:MET:HE2	2.02	0.42
2:B:234:LEU:HD13	2:B:239:TRP:HH2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:THR:C	1:A:475:GLN:H	2.28	0.42
1:A:134:SER:HG	1:A:139:THR:HG23	1.83	0.42
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.85	0.41
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.85	0.41
1:A:434:ILE:HD13	1:A:530:LYS:CB	2.50	0.41
2:B:335:GLY:HA2	2:B:367:GLN:OE1	2.20	0.41
2:B:94:ILE:HG12	2:B:161:GLN:NE2	2.35	0.41
1:A:257:ILE:HD13	1:A:282:LEU:HD12	2.03	0.41
1:A:450:THR:O	1:A:451:LYS:HB2	2.21	0.41
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.85	0.41
1:A:30:LYS:HG2	1:A:71:TRP:HZ3	1.82	0.41
2:B:85:GLN:HB2	2:B:154:LYS:HB2	2.03	0.41
2:B:160:PHE:CE2	2:B:164:MET:HE2	2.55	0.41
2:B:254:VAL:HG11	2:B:289:LEU:HA	2.00	0.41
1:A:50:ILE:O	1:A:143:ARG:HB2	2.20	0.41
1:A:395:LYS:HA	1:A:414:TRP:CH2	2.55	0.41
1:A:111:VAL:O	1:A:111:VAL:HG22	2.20	0.41
1:A:225:PRO:HA	1:A:226:PRO:C	2.46	0.41
2:B:353:LYS:O	2:B:353:LYS:HG3	2.17	0.41
1:A:291:GLU:HG3	1:A:293:ILE:HD11	2.03	0.41
1:A:298:GLU:N	1:A:298:GLU:CD	2.79	0.41
1:A:340:GLN:HG3	1:A:351:THR:HG22	2.02	0.41
2:B:282:LEU:HD13	2:B:282:LEU:HA	1.93	0.41
1:A:20:LYS:HG2	1:A:55:PRO:O	2.20	0.40
1:A:83:ARG:NH1	1:A:83:ARG:HG3	2.36	0.40
1:A:397:THR:HG21	1:A:424:LYS:HA	2.03	0.40
1:A:512:LYS:HD2	1:A:512:LYS:HA	1.73	0.40
2:B:121:ASP:O	2:B:125:ARG:HG3	2.20	0.40
2:B:349:LEU:N	2:B:349:LEU:HD22	2.36	0.40
2:B:238:LYS:H	2:B:238:LYS:HG2	1.52	0.40
2:B:293:ILE:O	2:B:293:ILE:HG22	2.21	0.40
1:A:116:PHE:HE2	1:A:146:TYR:HE1	1.69	0.40
1:A:277:ARG:HD3	1:A:334:GLN:HG3	2.02	0.40
1:A:500:GLN:H	1:A:500:GLN:HG2	1.67	0.40
2:B:362:THR:CG2	2:B:366:LYS:NZ	2.80	0.40
2:B:85:GLN:HG3	2:B:154:LYS:HB2	2.00	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	544/557 (98%)	507 (93%)	37 (7%)	0	100	100
2	B	403/428 (94%)	379 (94%)	24 (6%)	0	100	100
All	All	947/985 (96%)	886 (94%)	61 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	477/495 (96%)	421 (88%)	56 (12%)	5	11
2	B	364/390 (93%)	333 (92%)	31 (8%)	10	22
All	All	841/885 (95%)	754 (90%)	87 (10%)	7	15

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	27	THR
1	A	28	GLU
1	A	37	ILE
1	A	47	ILE
1	A	49	LYS
1	A	63	ILE
1	A	69	THR

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Mol	Chain	Res	Type
1	A	72	ARG
1	A	85	GLN
1	A	94	ILE
1	A	101	LYS
1	A	104	LYS
1	A	105	SER
1	A	111	VAL
1	A	130	PHE
1	A	131	THR
1	A	132	ILE
1	A	135	ILE
1	A	137	ASN
1	A	139	THR
1	A	148	VAL
1	A	169	GLU
1	A	177	ASP
1	A	178	ILE
1	A	186	ASP
1	A	193	LEU
1	A	204	GLU
1	A	216	THR
1	A	219	LYS
1	A	237	ASP
1	A	241	VAL
1	A	253	THR
1	A	261	VAL
1	A	283	LEU
1	A	284	ARG
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	300	GLU
1	A	334	GLN
1	A	347	LYS
1	A	349	LEU
1	A	366	LYS
1	A	396	GLU
1	A	409	THR
1	A	411	ILE
1	A	413	GLU
1	A	417	VAL
1	A	422	LEU

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Mol	Chain	Res	Type
1	A	448	ARG
1	A	471	ASN
1	A	473	THR
1	A	512	LYS
1	A	540	LYS
1	A	542	ILE
2	B	47	ILE
2	B	50	ILE
2	B	70	LYS
2	B	86	ASP
2	B	92	LEU
2	B	173	LYS
2	B	184	MET
2	B	187	LEU
2	B	200	THR
2	B	201	LYS
2	B	234	LEU
2	B	238	LYS
2	B	240	THR
2	B	248	GLU
2	B	268	SER
2	B	282	LEU
2	B	287	LYS
2	B	293	ILE
2	B	295	LEU
2	B	296	THR
2	B	297	GLU
2	B	301	LEU
2	B	330	GLN
2	B	349	LEU
2	B	353	LYS
2	B	356	ARG
2	B	361	HIS
2	B	370	GLU
2	B	418	ASN
2	B	423	VAL
2	B	425	LEU

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

Mol	Chain	Res	Type
1	A	57	ASN

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Mol	Chain	Res	Type
1	A	91	GLN
1	A	161	GLN
1	A	182	GLN
1	A	258	GLN
1	A	332	GLN
1	A	334	GLN
1	A	428	GLN
1	A	464	GLN
1	A	487	GLN
1	A	507	GLN
1	A	519	ASN
2	B	96	HIS
2	B	147	ASN
2	B	197	GLN
2	B	242	GLN
2	B	255	ASN
2	B	258	GLN
2	B	306	ASN

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](#)

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	X2G	A	601	-	32,35,36	2.23	8 (25%)	42,47,50	1.89	9 (21%)

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	X2G	A	601	-	-	2/15/18/19	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	X2G	C0P-N0H	8.21	1.49	1.37
3	A	601	X2G	C0K-N0H	5.83	1.45	1.37
3	A	601	X2G	C0O-C0N	4.30	1.53	1.43
3	A	601	X2G	O0S-C0N	-2.84	1.19	1.24
3	A	601	X2G	C0K-N0M	2.52	1.42	1.38
3	A	601	X2G	O0Q-C0K	-2.36	1.18	1.23
3	A	601	X2G	C0Y-C13	2.10	1.53	1.47
3	A	601	X2G	C0N-N0M	2.07	1.42	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	X2G	N0M-C0K-N0H	6.08	120.08	114.86
3	A	601	X2G	C0N-N0M-C0K	-5.38	119.93	126.61
3	A	601	X2G	C0O-C0N-N0M	3.66	119.93	114.80
3	A	601	X2G	O0Q-C0K-N0H	-3.35	120.03	122.87
3	A	601	X2G	O0S-C0N-C0O	-2.94	120.09	125.16
3	A	601	X2G	C0X-C0W-C0V	-2.89	119.99	123.50
3	A	601	X2G	C0O-C0P-N0H	-2.40	119.97	122.39
3	A	601	X2G	C0C-C0V-C0W	2.33	120.46	117.55
3	A	601	X2G	O0B-C05-C04	2.31	120.52	115.75

There are no chirality outliers.

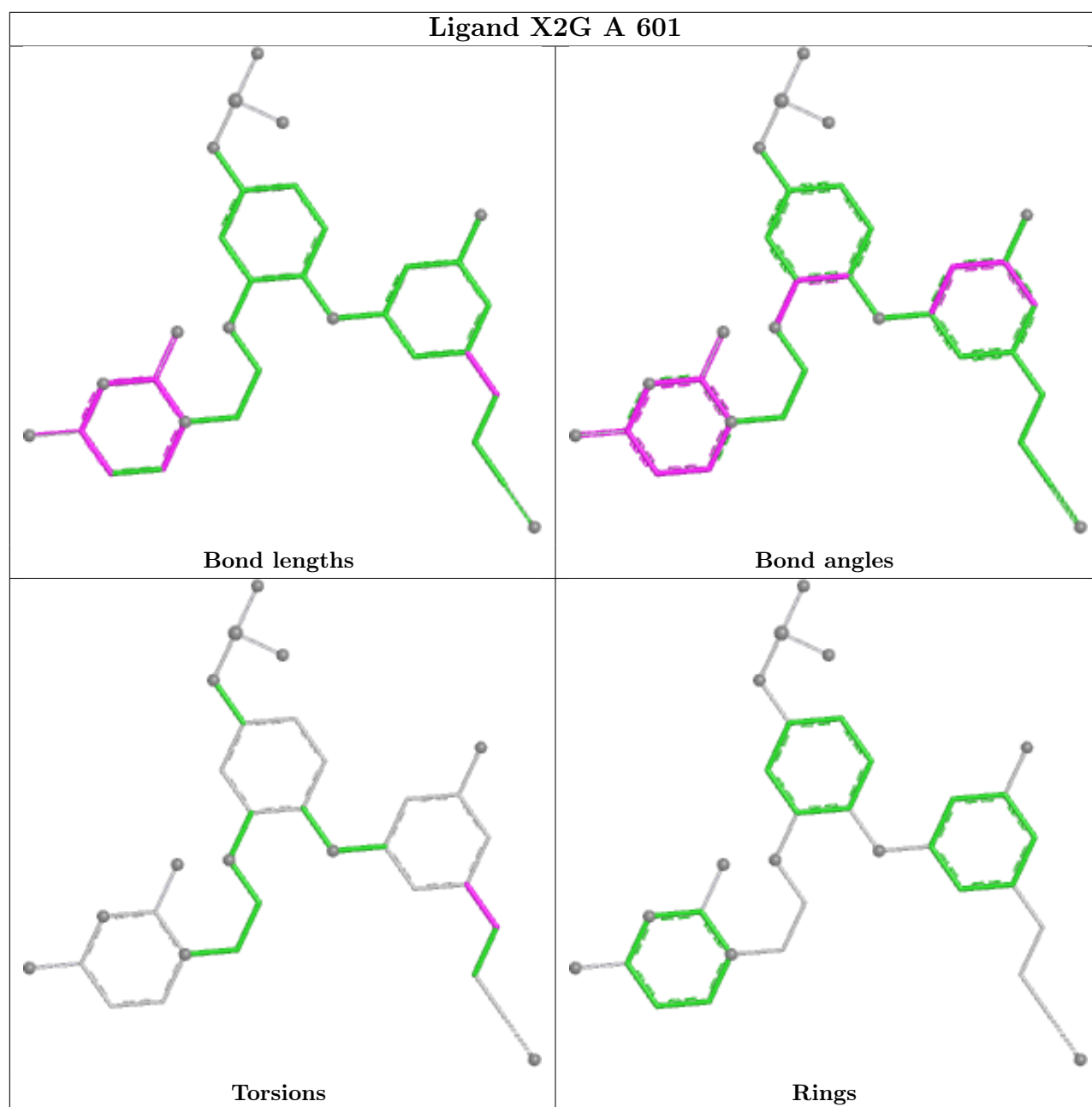
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	X2G	C0Z-C0Y-C13-C15
3	A	601	X2G	C0X-C0Y-C13-C15

There are no ring outliers.

No monomer is involved in short contacts.

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	548/557 (98%)	0.31	15 (2%) 56 50	69, 110, 161, 185	0
2	B	409/428 (95%)	0.23	10 (2%) 59 54	70, 99, 152, 199	0
All	All	957/985 (97%)	0.27	25 (2%) 57 51	69, 106, 157, 199	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	551	LEU	4.1
2	B	423	VAL	4.0
2	B	88	TRP	3.2
2	B	422	LEU	3.2
2	B	298	GLU	3.0
1	A	398	TRP	2.9
1	A	220	LYS	2.9
1	A	548	VAL	2.5
1	A	221	HIS	2.5
1	A	178	ILE	2.4
1	A	218	ASP	2.3
1	A	503	LEU	2.3
2	B	85	GLN	2.2
1	A	219	LYS	2.2
2	B	87	PHE	2.2
2	B	100	LEU	2.2
1	A	410	TRP	2.1
1	A	409	THR	2.1
1	A	543	GLY	2.1
1	A	135	ILE	2.1
2	B	232	TYR	2.1
1	A	181	TYR	2.0
1	A	223	LYS	2.0
2	B	299	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	188	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

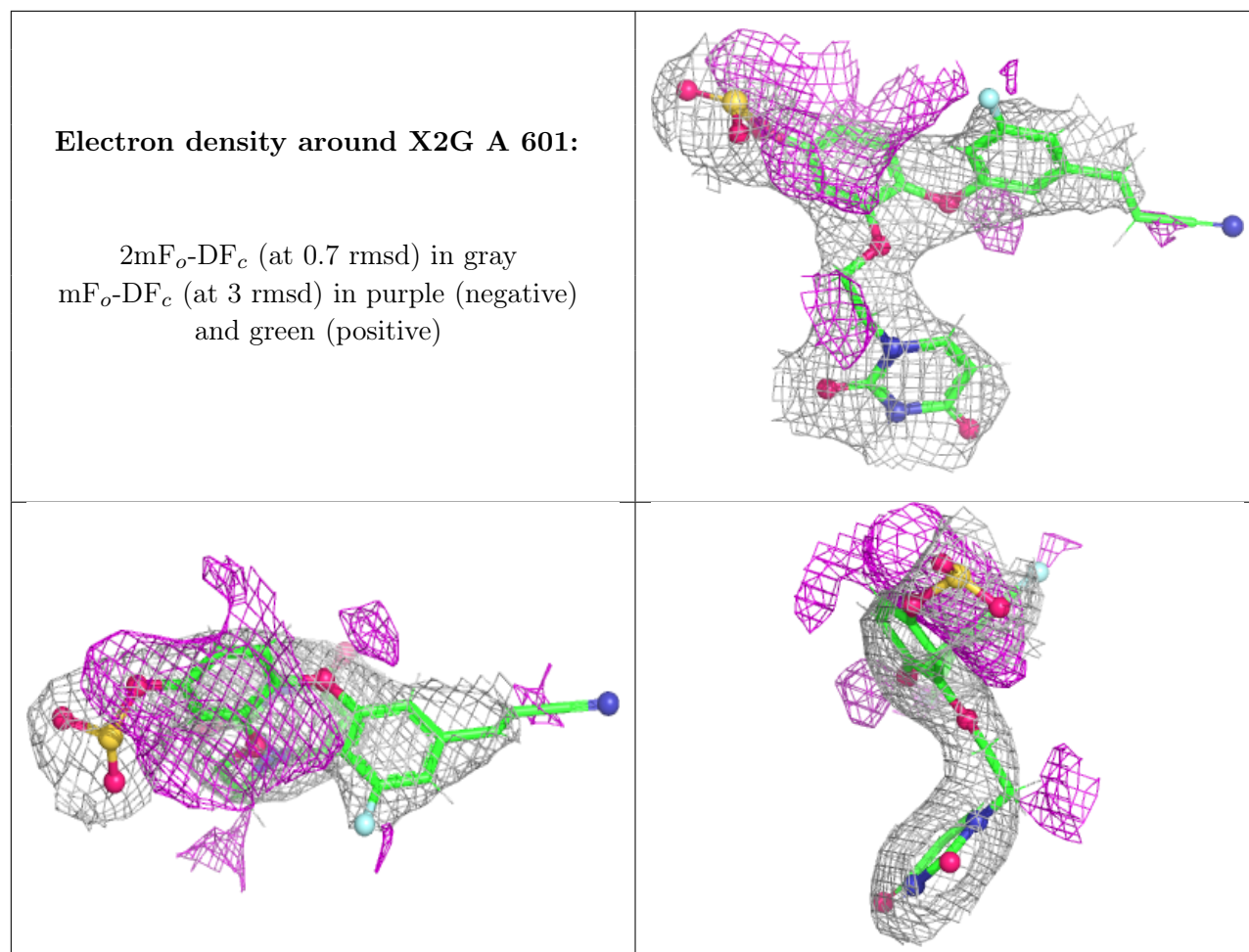
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	X2G	A	601	33/34	0.89	0.14	88,109,143,173	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.