



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2019 – 08:27 PM EST

PDB ID : 6C0N
Title : Crystal structure of HIV-1 reverse transcriptase in complex with non-nucleoside inhibitor 25a
Authors : Yang, Y.; Nguyen, L.A.; Smithline, Z.B.; Steitz, T.A.
Deposited on : 2018-01-01
Resolution : 2.00 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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

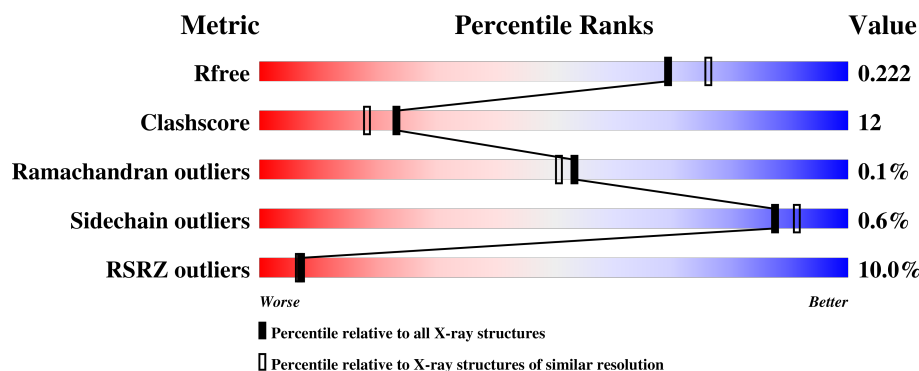
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

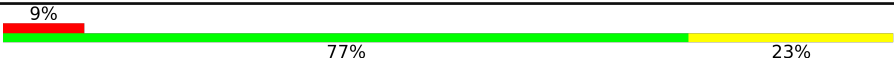

The reported resolution of this entry is 2.00 Å.

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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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. 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	 9% 77% 23%
2	B	428	 11% 75% 21% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	A	611	-	-	X	-
6	EDO	A	617	-	-	X	-
6	EDO	A	618	-	-	-	X
6	EDO	A	619	-	-	-	X
6	EDO	B	513	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8923 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	9	0
			4593	2975	763	846	9			

There are 5 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	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

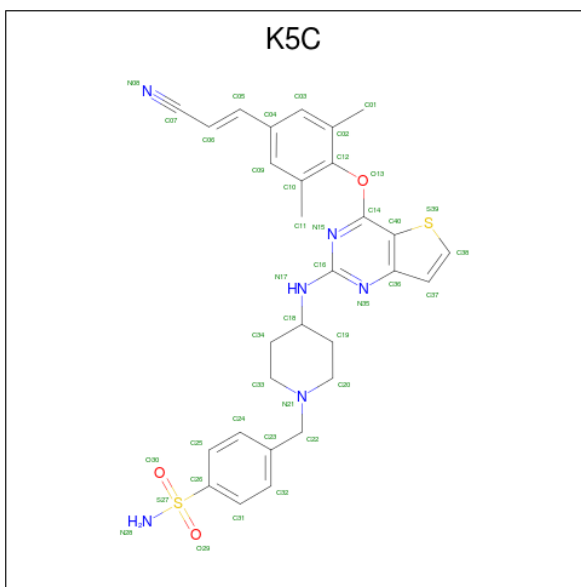
- Molecule 2 is a protein called Reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	7	0
			3465	2258	572	628	7			

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-({4-[(4-{4-[(E)-2-cyanoethenyl]-2,6-dimethylphenoxy}thieno[3,2-d]pyrimidin-2-yl)amino]piperidin-1-yl}methyl)benzene-1-sulfonamide (three-letter code: K5C) (formula: C₂₉H₃₀N₆O₃S₂) (labeled as "Ligand of Interest" by author).

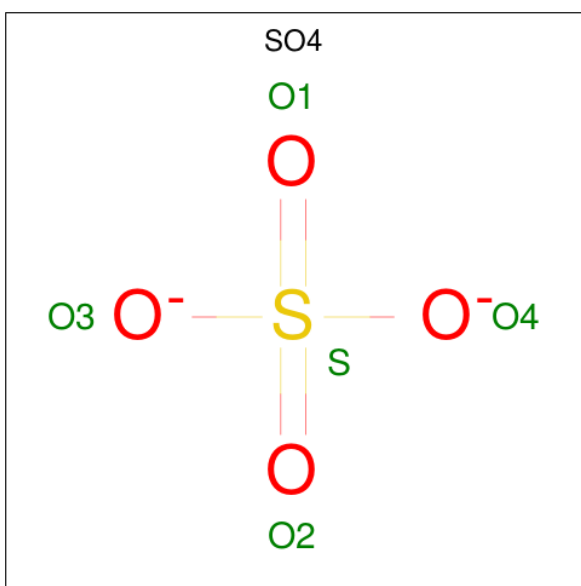


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			40	29	6	3	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

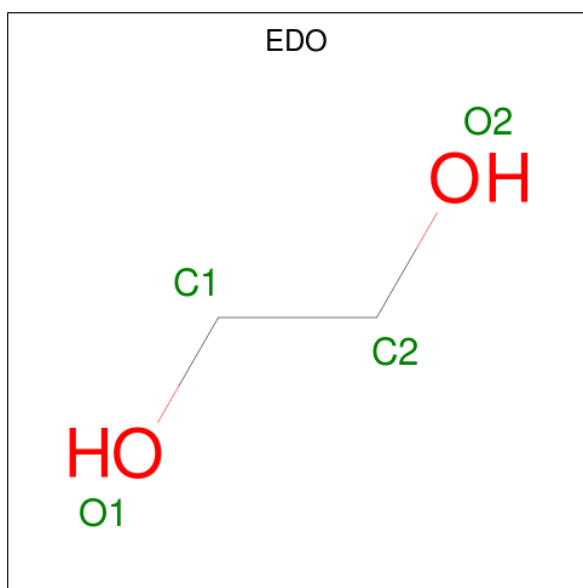
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



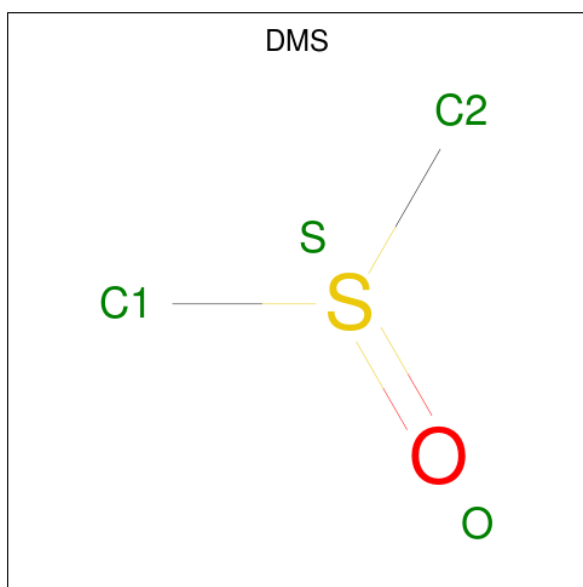
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	S	0	0
			4	2	1	1		

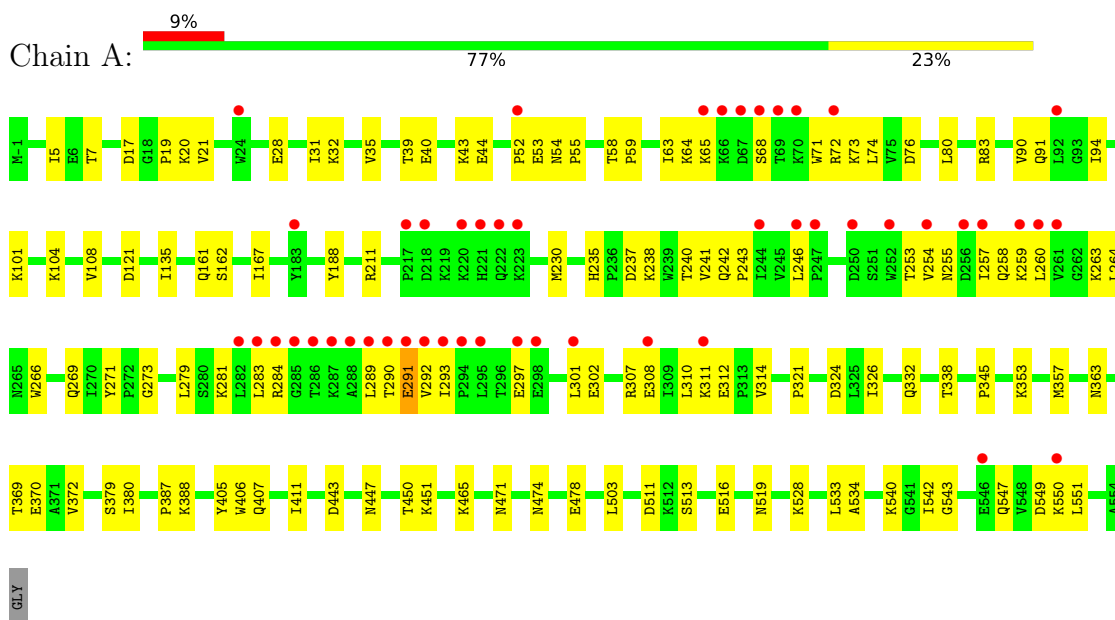
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	402	Total	O	0	0
			402	402		
8	B	290	Total	O	0	0
			290	290		

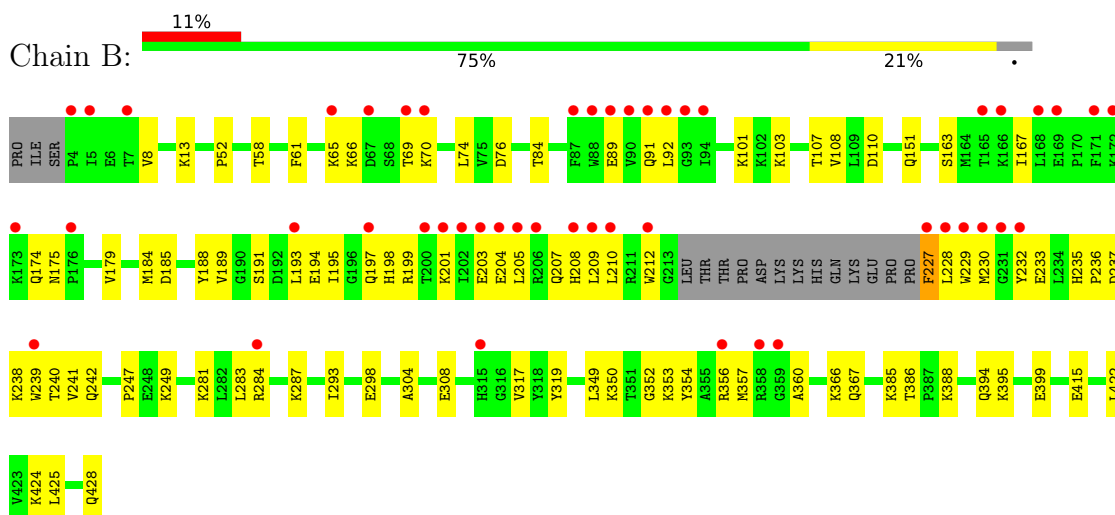
3 Residue-property plots [i](#)

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: Reverse transcriptase/ribonuclease H



• Molecule 2: 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	162.67Å 73.27Å 109.23Å 90.00° 100.12° 90.00°	Depositor
Resolution (Å)	48.78 – 2.00 48.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.78-2.00) 98.9 (48.78-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.181 , 0.222 0.181 , 0.222	Depositor DCC
R_{free} test set	4229 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8923	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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, DMS, K5C, EDO, SO4

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	0.35	0/4714	0.50	0/6409
2	B	0.38	0/3564	0.52	0/4839
All	All	0.37	0/8278	0.51	0/11248

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	4593	0	4648	119	0
2	B	3465	0	3493	84	0
3	A	40	0	0	0	0
4	A	1	0	0	0	0
5	A	20	0	0	1	0
5	B	20	0	0	0	0
6	A	56	0	84	19	0
6	B	32	0	48	7	0
7	B	4	0	6	2	0
8	A	402	0	0	9	0
8	B	290	0	0	12	0
All	All	8923	0	8279	201	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 12.

All (201) 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:551:LEU:HD21	6:A:618:EDO:H21	1.28	1.10
1:A:65:LYS:HB2	1:A:68:SER:HB2	1.38	1.05
1:A:388:LYS:HG3	6:A:617:EDO:H21	1.41	1.01
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.41	0.98
1:A:63:ILE:HB	1:A:72:ARG:HD3	1.47	0.94
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.53	0.91
1:A:332:GLN:NE2	1:A:338[A]:THR:HG23	1.95	0.80
2:B:353:LYS:H	6:B:509:EDO:H12	1.47	0.78
1:A:551:LEU:HD21	6:A:618:EDO:C2	2.12	0.77
2:B:70:LYS:HE2	8:B:843:HOH:O	1.86	0.75
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.71	0.72
2:B:195:ILE:O	2:B:199:ARG:HG2	1.89	0.72
1:A:338[A]:THR:HG22	8:A:809:HOH:O	1.89	0.72
2:B:110:ASP:HB3	2:B:228:LEU:CD2	2.20	0.71
2:B:110:ASP:HB3	2:B:228:LEU:HD22	1.73	0.71
1:A:388:LYS:CG	6:A:617:EDO:H21	2.21	0.71
2:B:394:GLN:HG3	8:B:738:HOH:O	1.89	0.70
1:A:543:GLY:HA3	2:B:283:LEU:O	1.90	0.70
1:A:353:LYS:H	6:A:611:EDO:H11	1.58	0.69
1:A:297:GLU:O	1:A:301:LEU:HD13	1.94	0.67
2:B:91:GLN:HG3	2:B:92:LEU:H	1.60	0.67
1:A:528:LYS:NZ	6:A:613:EDO:H11	2.09	0.67
2:B:386:THR:OG1	6:B:508:EDO:H12	1.95	0.66
1:A:547:GLN:O	1:A:550:LYS:HG2	1.95	0.66
1:A:63:ILE:HB	1:A:72:ARG:CD	2.23	0.65
2:B:101:LYS:O	2:B:236:PRO:HB2	1.96	0.65
1:A:551:LEU:CD2	6:A:618:EDO:H21	2.16	0.65
1:A:474:ASN:HB2	6:A:610:EDO:H11	1.78	0.65
2:B:69:THR:HA	8:B:797:HOH:O	1.95	0.65
1:A:528:LYS:HZ3	6:A:613:EDO:H11	1.62	0.64
2:B:354:TYR:CB	2:B:357:MET:HE2	2.27	0.64
2:B:191:SER:OG	2:B:198:HIS:ND1	2.28	0.64
1:A:406:TRP:N	6:A:615:EDO:H12	2.13	0.63
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.34	0.63
2:B:356:ARG:NH1	8:B:602:HOH:O	2.28	0.63
1:A:503:LEU:HD23	2:B:422:LEU:HD13	1.79	0.63
8:A:947:HOH:O	2:B:424:LYS:HD2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HE3	1:A:284:ARG:NH2	2.13	0.62
2:B:193:LEU:HD13	2:B:197:GLN:HB3	1.80	0.62
1:A:388:LYS:HE3	6:A:617:EDO:C2	2.31	0.61
1:A:353:LYS:H	6:A:611:EDO:C1	2.14	0.61
1:A:28:GLU:O	1:A:32:LYS:HG2	2.01	0.61
2:B:167:ILE:HG23	2:B:212:TRP:CG	2.36	0.60
2:B:281:LYS:O	2:B:284:ARG:HG2	2.01	0.60
2:B:317:VAL:CG1	2:B:349:LEU:HD23	2.31	0.60
1:A:273:GLY:HA2	1:A:338[A]:THR:HG21	1.83	0.60
2:B:353:LYS:H	6:B:509:EDO:C1	2.14	0.59
1:A:547:GLN:HA	1:A:550:LYS:HE3	1.85	0.59
2:B:228:LEU:HD23	8:B:604:HOH:O	2.02	0.59
2:B:354:TYR:HB3	2:B:357:MET:HE2	1.84	0.58
2:B:184:MET:HE3	8:B:773:HOH:O	2.03	0.58
2:B:91:GLN:HG3	2:B:92:LEU:N	2.17	0.58
1:A:108:VAL:HG22	1:A:188:TYR:CD2	2.39	0.58
1:A:237:ASP:O	1:A:238:LYS:HD3	2.05	0.57
1:A:478:GLU:HG2	8:A:898:HOH:O	2.03	0.57
1:A:242:GLN:HB3	1:A:243:PRO:HD2	1.85	0.57
1:A:259:LYS:NZ	1:A:263:LYS:HE3	2.19	0.57
2:B:191:SER:HG	2:B:198:HIS:HD1	1.40	0.57
2:B:388:LYS:HE3	2:B:415:GLU:OE1	2.05	0.57
1:A:451:LYS:HB3	1:A:471:ASN:HA	1.87	0.57
2:B:425:LEU:O	2:B:428:GLN:HB2	2.04	0.57
1:A:253:THR:HG22	1:A:292:VAL:HG12	1.88	0.56
2:B:8:VAL:HG11	2:B:89:GLU:OE2	2.05	0.55
2:B:205:LEU:O	2:B:209:LEU:HG	2.07	0.55
1:A:406:TRP:H	6:A:615:EDO:H12	1.70	0.55
1:A:101:LYS:HD3	1:A:321:PRO:CG	2.37	0.55
2:B:163:SER:O	2:B:167:ILE:HG13	2.07	0.55
1:A:63:ILE:HG22	1:A:64:LYS:H	1.71	0.55
1:A:271:TYR:CE2	1:A:314[B]:VAL:HG12	2.42	0.54
1:A:20[B]:LYS:NZ	1:A:55:PRO:HB2	2.23	0.54
1:A:63:ILE:O	1:A:72:ARG:HG2	2.07	0.54
1:A:20[B]:LYS:HZ1	1:A:55:PRO:HB2	1.73	0.53
2:B:195:ILE:HG12	2:B:199:ARG:HD3	1.90	0.53
2:B:360:ALA:HB2	2:B:366:LYS:CD	2.26	0.53
1:A:550:LYS:HD2	8:A:955:HOH:O	2.09	0.53
1:A:73:LYS:NZ	5:A:603:SO4:O4	2.23	0.53
1:A:31:ILE:O	1:A:35:VAL:HG23	2.08	0.52
1:A:503:LEU:CD2	2:B:422:LEU:HD13	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PRO:HA	8:A:715:HOH:O	2.09	0.52
2:B:65:LYS:NZ	8:B:607:HOH:O	2.40	0.52
2:B:58:THR:HG23	2:B:76:ASP:O	2.10	0.52
2:B:151:GLN:NE2	8:B:619:HOH:O	2.43	0.51
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.41	0.51
2:B:239:TRP:HB3	2:B:350:LYS:HE2	1.92	0.51
1:A:372:VAL:HG11	1:A:411[A]:ILE:HD12	1.93	0.51
2:B:110:ASP:HB3	2:B:228:LEU:HD23	1.93	0.51
2:B:204:GLU:O	2:B:204:GLU:HG2	2.10	0.51
2:B:13:LYS:HE3	2:B:84:THR:O	2.11	0.51
1:A:332:GLN:CD	1:A:338[A]:THR:HG23	2.31	0.51
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.46	0.51
1:A:372:VAL:HG11	1:A:411[A]:ILE:HG23	1.93	0.51
1:A:326[B]:ILE:HD13	1:A:388:LYS:HB2	1.93	0.51
1:A:290:THR:O	1:A:290:THR:HG22	2.12	0.50
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.94	0.50
2:B:242:GLN:NE2	8:B:601:HOH:O	2.26	0.49
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.12	0.49
1:A:311:LYS:HG3	1:A:312:GLU:HG3	1.95	0.49
1:A:533:LEU:O	6:A:616:EDO:H12	2.13	0.49
1:A:388:LYS:HE3	6:A:617:EDO:H21	1.95	0.49
1:A:254:VAL:O	1:A:258:GLN:HG3	2.12	0.49
2:B:228:LEU:O	2:B:229:TRP:HB3	2.12	0.49
1:A:53:GLU:HG2	1:A:54:ASN:N	2.28	0.49
1:A:64:LYS:HE3	1:A:71:TRP:CD2	2.48	0.49
2:B:210:LEU:HD22	2:B:227:PHE:CZ	2.48	0.49
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.95	0.48
1:A:161:GLN:HG2	8:A:748:HOH:O	2.12	0.48
1:A:39:THR:O	1:A:43:LYS:HG3	2.13	0.48
2:B:240:THR:OG1	2:B:241:VAL:N	2.46	0.48
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.43	0.48
1:A:292:VAL:O	1:A:292:VAL:HG23	2.14	0.47
1:A:281:LYS:O	1:A:284:ARG:HG3	2.14	0.47
1:A:308:GLU:O	1:A:311:LYS:HG2	2.14	0.47
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.49	0.47
2:B:189:VAL:HG21	2:B:205:LEU:HD23	1.96	0.47
2:B:354:TYR:HB2	2:B:357:MET:HE2	1.94	0.47
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.97	0.47
1:A:253:THR:HA	1:A:292:VAL:HA	1.96	0.47
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.50	0.47
1:A:63:ILE:C	1:A:72:ARG:HG2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:GLU:CD	2:B:233:GLU:H	2.18	0.47
1:A:353:LYS:O	6:A:611:EDO:H12	2.15	0.46
2:B:195:ILE:HG12	2:B:199:ARG:CD	2.45	0.46
1:A:534:ALA:HA	6:A:616:EDO:H12	1.97	0.46
2:B:174:GLN:HG3	2:B:175:ASN:OD1	2.16	0.46
1:A:63:ILE:CB	1:A:72:ARG:HD3	2.32	0.46
1:A:90:VAL:O	1:A:90:VAL:HG22	2.15	0.46
1:A:443:ASP:OD2	1:A:549:ASP:HA	2.16	0.46
7:B:501:DMS:H12	8:B:614:HOH:O	2.16	0.46
1:A:94:ILE:HG21	1:A:230:MET:HE2	1.98	0.46
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.16	0.45
2:B:208:HIS:O	2:B:212:TRP:HD1	1.99	0.45
2:B:228:LEU:HD23	2:B:230:MET:HB3	1.97	0.45
2:B:287:LYS:HD3	2:B:293:ILE:HD11	1.97	0.45
1:A:290:THR:O	1:A:290:THR:CG2	2.64	0.45
1:A:380:ILE:CD1	7:B:501:DMS:H22	2.46	0.45
1:A:5:ILE:HG12	1:A:167:ILE:HD11	1.98	0.45
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.98	0.45
1:A:357:MET:HE2	1:A:370:GLU:OE2	2.17	0.45
1:A:40:GLU:O	1:A:44:GLU:HG3	2.16	0.45
1:A:240:THR:HG23	1:A:241:VAL:O	2.16	0.45
2:B:247:PRO:HB2	2:B:249[A]:LYS:HD2	1.99	0.45
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.16	0.45
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.99	0.45
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.52	0.45
2:B:352:GLY:HA3	6:B:509:EDO:H11	1.99	0.45
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.98	0.45
1:A:63:ILE:HD11	1:A:74:LEU:HD13	1.98	0.45
1:A:101:LYS:HB2	8:A:787:HOH:O	2.16	0.44
2:B:298:GLU:CD	2:B:298:GLU:H	2.18	0.44
2:B:91:GLN:CG	2:B:92:LEU:H	2.28	0.44
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.78	0.44
2:B:195:ILE:CG1	2:B:199:ARG:HD3	2.47	0.44
2:B:235:HIS:C	2:B:237:ASP:H	2.20	0.44
1:A:63:ILE:HG22	1:A:64:LYS:N	2.32	0.44
2:B:203:GLU:O	2:B:207:GLN:HG2	2.18	0.44
1:A:104:LYS:HE3	1:A:104:LYS:HB2	1.77	0.44
1:A:7:THR:HG21	1:A:121:ASP:HA	1.98	0.44
2:B:304:ALA:O	2:B:308:GLU:HG2	2.18	0.44
1:A:39:THR:HG22	1:A:43:LYS:HE3	2.00	0.44
1:A:94:ILE:HD13	1:A:230:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:NZ	8:A:720:HOH:O	2.47	0.43
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.01	0.43
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.99	0.43
1:A:516:GLU:HA	1:A:516:GLU:OE1	2.19	0.43
1:A:513:SER:N	1:A:519:ASN:OD1	2.51	0.43
1:A:379:SER:CB	1:A:387:PRO:HD3	2.48	0.43
1:A:53:GLU:HG2	1:A:54:ASN:H	1.84	0.43
2:B:354:TYR:CD2	2:B:357:MET:HE1	2.54	0.43
2:B:395:LYS:O	2:B:399[B]:GLU:HG3	2.19	0.43
2:B:228:LEU:CD2	2:B:230:MET:HB3	2.47	0.43
1:A:235:HIS:HB2	1:A:238:LYS:O	2.19	0.43
1:A:63:ILE:HB	1:A:72:ARG:CG	2.48	0.43
1:A:345:PRO:HA	8:A:797:HOH:O	2.19	0.43
1:A:65:LYS:HB3	1:A:65:LYS:HE3	1.86	0.43
2:B:179:VAL:HA	8:B:647:HOH:O	2.19	0.42
1:A:162[B]:SER:OG	2:B:52:PRO:HG3	2.18	0.42
1:A:101:LYS:HD3	1:A:321:PRO:HG2	2.02	0.42
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.20	0.42
1:A:369:THR:HA	1:A:411[A]:ILE:HD11	2.00	0.42
2:B:66:LYS:HZ1	6:B:510:EDO:H21	1.84	0.42
1:A:259:LYS:NZ	1:A:263:LYS:HG3	2.34	0.42
1:A:266:TRP:O	1:A:269:GLN:HG2	2.19	0.42
1:A:450:THR:O	1:A:451:LYS:HB2	2.19	0.42
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.83	0.42
1:A:259:LYS:HZ1	1:A:263:LYS:HE3	1.83	0.42
1:A:28:GLU:HG3	1:A:135:ILE:CD1	2.46	0.42
1:A:291:GLU:O	1:A:293:ILE:HG13	2.19	0.42
2:B:357:MET:HB2	2:B:367:GLN:HG2	2.02	0.41
2:B:107:THR:HA	2:B:232:TYR:O	2.20	0.41
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.20	0.41
1:A:260:LEU:O	1:A:264:LEU:HG	2.20	0.41
1:A:324:ASP:OD1	6:A:617:EDO:H11	2.20	0.41
2:B:91:GLN:CG	2:B:92:LEU:N	2.84	0.41
1:A:58:THR:HG23	1:A:76:ASP:O	2.21	0.41
6:B:512:EDO:H21	8:B:754:HOH:O	2.20	0.41
1:A:353:LYS:N	6:A:611:EDO:H11	2.31	0.41
1:A:17:ASP:O	1:A:83:ARG:HD3	2.21	0.41
2:B:210:LEU:HD22	2:B:227:PHE:CE2	2.56	0.40
2:B:229:TRP:CG	2:B:229:TRP:O	2.74	0.40
1:A:94:ILE:HD13	1:A:230:MET:HE3	2.02	0.40
2:B:66:LYS:NZ	6:B:510:EDO:H21	2.37	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	563/557 (101%)	548 (97%)	14 (2%)	1 (0%)	49	46
2	B	415/428 (97%)	396 (95%)	19 (5%)	0	100	100
All	All	978/985 (99%)	944 (96%)	33 (3%)	1 (0%)	53	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLU

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	504/495 (102%)	502 (100%)	2 (0%)	92	94
2	B	381/390 (98%)	378 (99%)	3 (1%)	83	87
All	All	885/885 (100%)	880 (99%)	5 (1%)	87	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	211	ARG

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Mol	Chain	Res	Type
2	B	194	GLU
2	B	227	PHE
2	B	238	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	394	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 1 is monoatomic - leaving 32 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	$\# Z > 2$
3	K5C	A	601	-	43,44,44	1.19	3 (6%)	52,63,63	2.16	16 (30%)
5	SO4	A	603	-	4,4,4	0.16	0	6,6,6	0.10	0
5	SO4	A	604	-	4,4,4	0.17	0	6,6,6	0.20	0
5	SO4	A	605	-	4,4,4	0.16	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	606	-	4,4,4	0.16	0	6,6,6	0.16	0
6	EDO	A	607	-	3,3,3	0.49	0	2,2,2	0.30	0
6	EDO	A	608	-	3,3,3	0.50	0	2,2,2	0.25	0
6	EDO	A	609	-	3,3,3	0.47	0	2,2,2	0.40	0
6	EDO	A	610	-	3,3,3	0.45	0	2,2,2	0.46	0
6	EDO	A	611	-	3,3,3	0.46	0	2,2,2	0.31	0
6	EDO	A	612	-	3,3,3	0.41	0	2,2,2	0.55	0
6	EDO	A	613	-	3,3,3	0.50	0	2,2,2	0.34	0
6	EDO	A	614	-	3,3,3	0.49	0	2,2,2	0.24	0
6	EDO	A	615	-	3,3,3	0.48	0	2,2,2	0.35	0
6	EDO	A	616	-	3,3,3	0.50	0	2,2,2	0.17	0
6	EDO	A	617	-	3,3,3	0.46	0	2,2,2	0.25	0
6	EDO	A	618	-	3,3,3	0.48	0	2,2,2	0.26	0
6	EDO	A	619	-	3,3,3	0.45	0	2,2,2	0.40	0
6	EDO	A	620	-	3,3,3	0.43	0	2,2,2	0.45	0
7	DMS	B	501	-	3,3,3	0.68	0	3,3,3	0.72	0
5	SO4	B	502	-	4,4,4	0.17	0	6,6,6	0.06	0
5	SO4	B	503	-	4,4,4	0.16	0	6,6,6	0.09	0
5	SO4	B	504	-	4,4,4	0.16	0	6,6,6	0.05	0
5	SO4	B	505	-	4,4,4	0.15	0	6,6,6	0.06	0
6	EDO	B	506	-	3,3,3	0.55	0	2,2,2	0.05	0
6	EDO	B	507	-	3,3,3	0.46	0	2,2,2	0.32	0
6	EDO	B	508	-	3,3,3	0.54	0	2,2,2	0.24	0
6	EDO	B	509	-	3,3,3	0.50	0	2,2,2	0.25	0
6	EDO	B	510	-	3,3,3	0.47	0	2,2,2	0.41	0
6	EDO	B	511	-	3,3,3	0.52	0	2,2,2	0.24	0
6	EDO	B	512	-	3,3,3	0.43	0	2,2,2	0.47	0
6	EDO	B	513	-	3,3,3	0.45	0	2,2,2	0.37	0

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	K5C	A	601	-	-	6/21/32/32	0/5/5/5
6	EDO	A	607	-	-	0/1/1/1	-
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	A	609	-	-	1/1/1/1	-
6	EDO	A	610	-	-	0/1/1/1	-
6	EDO	A	611	-	-	0/1/1/1	-
6	EDO	A	612	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	613	-	-	1/1/1/1	-
6	EDO	A	614	-	-	0/1/1/1	-
6	EDO	A	615	-	-	0/1/1/1	-
6	EDO	A	616	-	-	0/1/1/1	-
6	EDO	A	617	-	-	0/1/1/1	-
6	EDO	A	618	-	-	0/1/1/1	-
6	EDO	A	619	-	-	0/1/1/1	-
6	EDO	A	620	-	-	0/1/1/1	-
6	EDO	B	506	-	-	0/1/1/1	-
6	EDO	B	507	-	-	0/1/1/1	-
6	EDO	B	508	-	-	0/1/1/1	-
6	EDO	B	509	-	-	1/1/1/1	-
6	EDO	B	510	-	-	0/1/1/1	-
6	EDO	B	511	-	-	1/1/1/1	-
6	EDO	B	512	-	-	0/1/1/1	-
6	EDO	B	513	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	K5C	C16-N17	2.81	1.38	1.34
3	A	601	K5C	S27-N28	2.71	1.66	1.60
3	A	601	K5C	C20-N21	2.29	1.53	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	K5C	C16-N17-C18	5.75	129.95	123.59
3	A	601	K5C	C31-C26-C25	-5.54	112.64	120.43
3	A	601	K5C	C32-C31-C26	5.45	125.15	119.45
3	A	601	K5C	C22-N21-C20	-4.64	101.03	111.04
3	A	601	K5C	C24-C25-C26	4.47	124.12	119.45
3	A	601	K5C	O29-S27-C26	3.20	111.01	107.36
3	A	601	K5C	O13-C14-C40	3.12	121.07	115.69
3	A	601	K5C	C31-C26-S27	2.97	124.21	119.74
3	A	601	K5C	O30-S27-O29	-2.70	114.14	118.73
3	A	601	K5C	C01-C02-C03	2.58	124.28	119.49
3	A	601	K5C	C09-C04-C03	-2.50	115.68	119.11
3	A	601	K5C	C22-C23-C32	2.49	125.48	120.77
3	A	601	K5C	O13-C14-N15	-2.39	115.52	119.68
3	A	601	K5C	C25-C26-S27	2.27	123.15	119.74
3	A	601	K5C	C33-N21-C20	2.25	113.82	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	K5C	C34-C18-C19	2.10	114.55	110.84

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	K5C	C03-C04-C05-C06
3	A	601	K5C	C09-C04-C05-C06
6	A	613	EDO	O1-C1-C2-O2
6	B	509	EDO	O1-C1-C2-O2
6	B	511	EDO	O1-C1-C2-O2
3	A	601	K5C	C25-C26-S27-O29
3	A	601	K5C	C31-C26-S27-O29
3	A	601	K5C	C25-C26-S27-N28
6	A	609	EDO	O1-C1-C2-O2
3	A	601	K5C	C31-C26-S27-N28

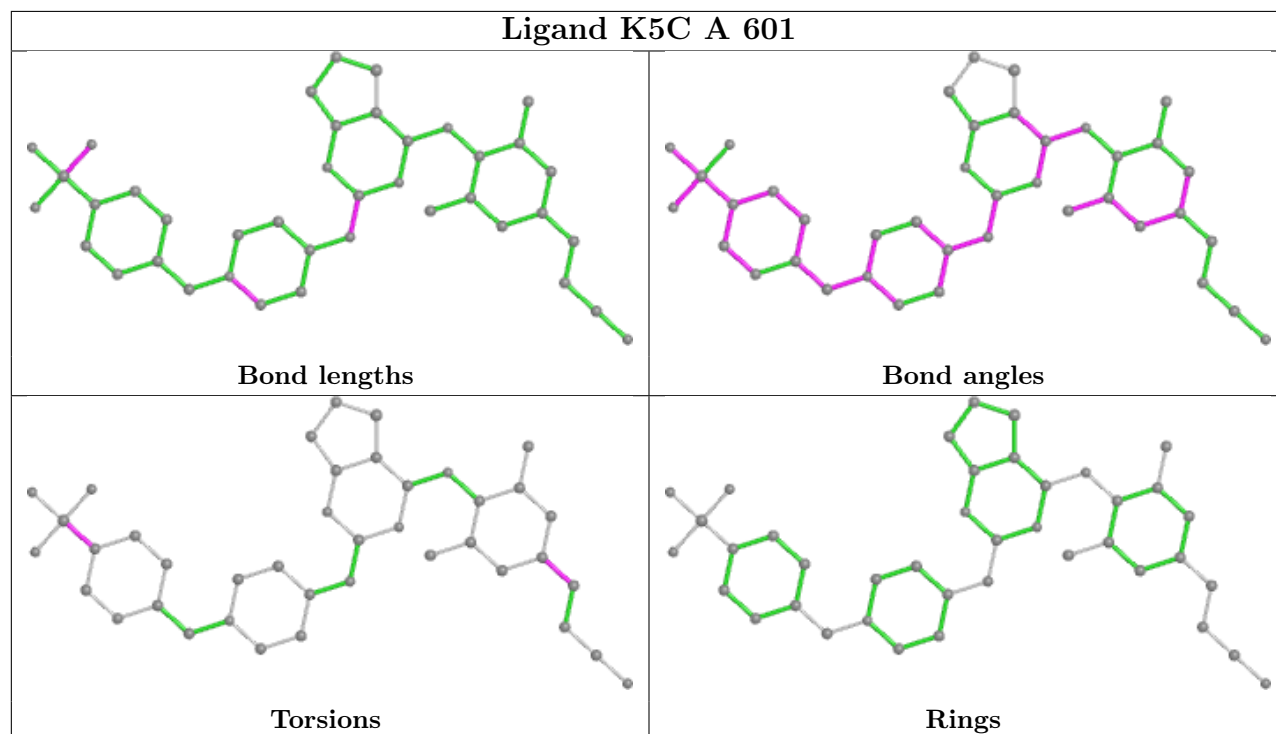
There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	610	EDO	1	0
6	A	611	EDO	4	0
6	A	613	EDO	2	0
6	A	615	EDO	2	0
6	A	616	EDO	2	0
6	A	617	EDO	5	0
6	A	618	EDO	3	0
6	B	508	EDO	1	0
6	B	509	EDO	3	0
6	B	510	EDO	2	0
6	B	512	EDO	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 [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	556/557 (99%)	0.47	49 (8%)	10 9	42, 69, 149, 243	0
2	B	412/428 (96%)	0.69	48 (11%)	4 4	39, 66, 144, 252	0
All	All	968/985 (98%)	0.57	97 (10%)	7 7	39, 68, 148, 252	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	90	VAL	14.2
1	A	67	ASP	12.7
2	B	89	GLU	9.7
1	A	257	ILE	8.6
1	A	286	THR	8.3
2	B	230	MET	8.1
2	B	91	GLN	7.4
1	A	290	THR	7.4
2	B	227	PHE	7.3
1	A	246	LEU	7.0
1	A	66	LYS	7.0
2	B	92	LEU	6.7
1	A	292	VAL	6.6
1	A	301	LEU	6.6
2	B	197	GLN	6.5
1	A	68	SER	6.4
1	A	295	LEU	5.9
2	B	4	PRO	5.8
2	B	229	TRP	5.7
2	B	209	LEU	5.6
1	A	288	ALA	5.5
2	B	202	ILE	5.4
1	A	293	ILE	5.4
1	A	252	TRP	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	294	PRO	5.4
1	A	260	LEU	5.3
1	A	282	LEU	5.3
1	A	289	LEU	5.3
1	A	223	LYS	5.2
1	A	69	THR	5.1
1	A	254	VAL	5.0
2	B	212	TRP	4.9
2	B	166	LYS	4.7
1	A	297	GLU	4.4
2	B	169	GLU	4.4
2	B	88	TRP	4.2
2	B	228	LEU	4.2
1	A	92	LEU	4.2
2	B	359	GLY	4.1
2	B	232	TYR	4.1
1	A	72	ARG	4.0
2	B	206	ARG	4.0
2	B	67	ASP	3.9
2	B	168	LEU	3.8
2	B	231	GLY	3.8
1	A	218	ASP	3.7
1	A	65	LYS	3.7
2	B	205	LEU	3.6
2	B	5	ILE	3.6
1	A	220	LYS	3.6
2	B	69	THR	3.6
2	B	358	ARG	3.6
1	A	221	HIS	3.5
2	B	193	LEU	3.3
1	A	217	PRO	3.3
2	B	239	TRP	3.3
2	B	165	THR	3.3
1	A	283	LEU	3.3
2	B	210	LEU	3.2
1	A	298	GLU	3.2
1	A	256	ASP	3.2
2	B	87	PHE	3.1
2	B	208	HIS	3.1
2	B	204	GLU	3.1
1	A	287	LYS	3.1
1	A	291	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	172	LYS	2.9
2	B	173	LYS	2.9
2	B	65	LYS	2.9
1	A	259	LYS	2.8
1	A	546	GLU	2.8
1	A	244	ILE	2.8
2	B	7	THR	2.8
1	A	550	LYS	2.7
2	B	284	ARG	2.7
1	A	284	ARG	2.7
2	B	356	ARG	2.7
2	B	200	THR	2.7
2	B	93	GLY	2.7
1	A	222	GLN	2.6
2	B	201	LYS	2.6
1	A	250	ASP	2.6
2	B	70	LYS	2.6
1	A	52	PRO	2.6
2	B	315	HIS	2.5
2	B	94	ILE	2.5
2	B	203	GLU	2.5
1	A	285	GLY	2.5
1	A	247	PRO	2.4
1	A	308	GLU	2.3
1	A	70	LYS	2.3
1	A	24	TRP	2.3
1	A	311	LYS	2.3
2	B	176	PRO	2.2
1	A	261	VAL	2.2
1	A	183	TYR	2.2
2	B	171	PHE	2.1

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 carbohydrates in this entry.

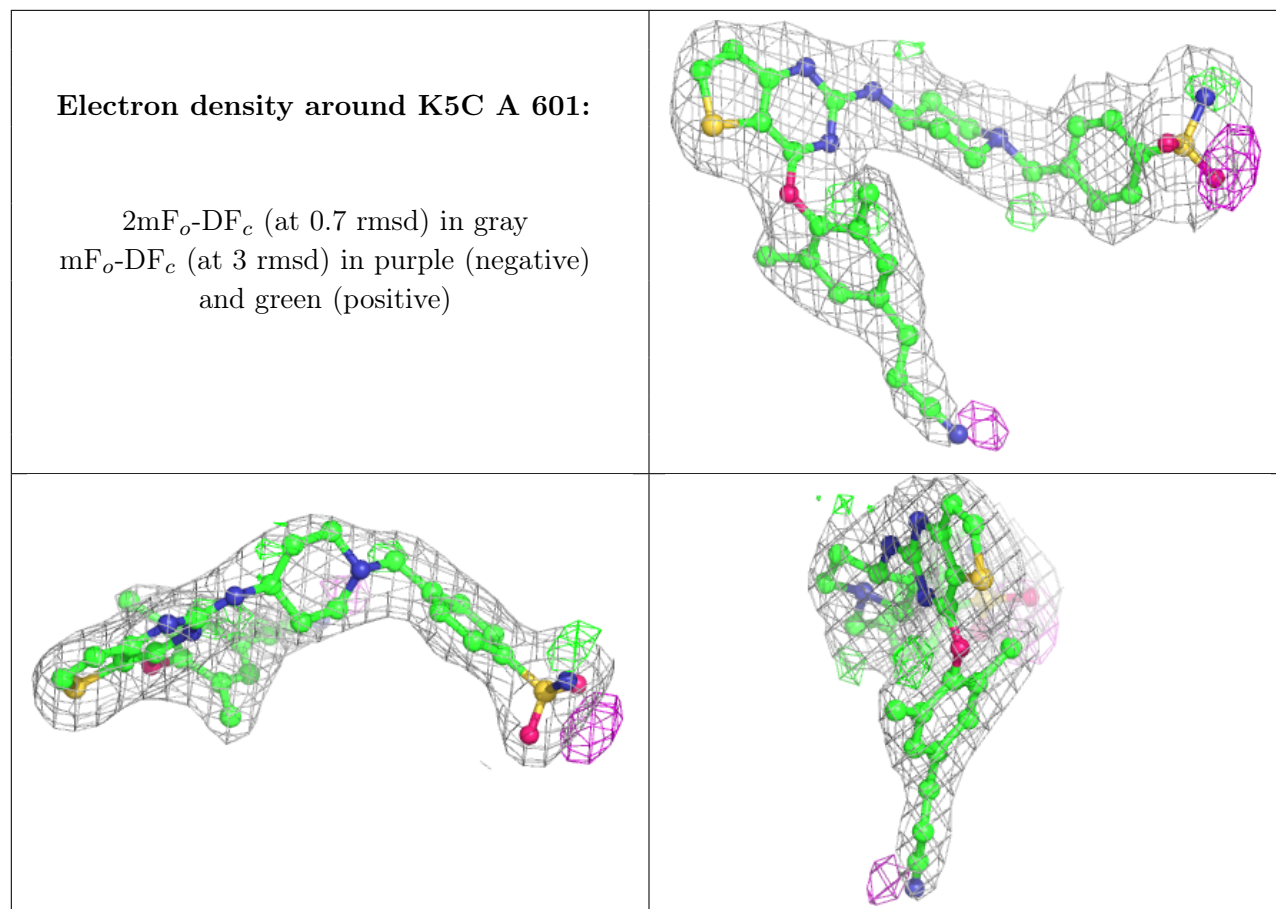
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	618	4/4	0.51	0.56	126,126,126,126	4
6	EDO	B	511	4/4	0.55	0.39	96,98,101,102	0
6	EDO	B	509	4/4	0.62	0.36	103,104,104,107	0
6	EDO	B	508	4/4	0.67	0.21	86,88,89,89	0
6	EDO	B	513	4/4	0.68	0.49	132,135,139,142	0
6	EDO	A	609	4/4	0.71	0.21	76,78,82,85	0
6	EDO	A	613	4/4	0.77	0.15	70,70,74,81	0
6	EDO	A	620	4/4	0.78	0.28	102,105,110,116	0
6	EDO	A	619	4/4	0.79	0.43	123,124,126,126	0
6	EDO	A	607	4/4	0.79	0.17	94,95,97,99	0
6	EDO	A	608	4/4	0.79	0.32	104,105,107,110	0
6	EDO	A	617	4/4	0.82	0.25	94,97,99,100	0
6	EDO	A	611	4/4	0.83	0.17	85,87,92,92	0
6	EDO	B	510	4/4	0.84	0.26	103,103,104,105	0
4	MG	A	602	1/1	0.85	0.26	80,80,80,80	0
6	EDO	A	616	4/4	0.85	0.24	74,81,90,96	0
6	EDO	A	610	4/4	0.87	0.13	73,75,79,88	0
5	SO4	B	505	5/5	0.89	0.27	142,142,143,143	0
6	EDO	B	506	4/4	0.89	0.24	61,68,76,76	0
6	EDO	A	615	4/4	0.89	0.32	93,96,103,107	0
5	SO4	B	502	5/5	0.90	0.23	142,143,146,149	0
5	SO4	A	605	5/5	0.91	0.15	113,117,120,121	0
5	SO4	B	504	5/5	0.92	0.28	147,147,149,149	0
5	SO4	B	503	5/5	0.92	0.31	160,160,162,163	0
6	EDO	B	512	4/4	0.93	0.32	109,110,110,112	0
3	K5C	A	601	40/40	0.93	0.12	53,67,97,100	0
6	EDO	A	614	4/4	0.94	0.15	86,88,91,95	0
6	EDO	B	507	4/4	0.94	0.19	62,65,73,77	0
5	SO4	A	606	5/5	0.94	0.22	111,112,115,119	0
6	EDO	A	612	4/4	0.94	0.20	55,60,69,72	0
5	SO4	A	603	5/5	0.95	0.14	121,123,124,128	0
5	SO4	A	604	5/5	0.96	0.10	98,101,104,111	0
7	DMS	B	501	4/4	0.98	0.17	59,70,72,78	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.