



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 09:38 PM BST

PDB ID : 6CGF
Title : Crystal structure of HIV-1 Y188L mutant reverse transcriptase in complex with non-nucleoside inhibitor K-5a2
Authors : Yang, Y.; Nguyen, L.A.; Smithline, Z.B.; Steitz, T.A.
Deposited on : 2018-02-20
Resolution : 1.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

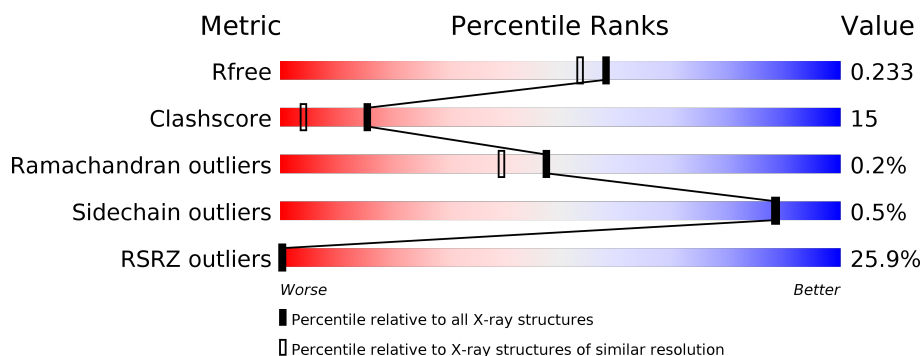
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	557	<div> <div>26%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>
2	B	428	<div> <div>25%</div> <div>77%</div> <div>19%</div> <div>.</div> </div>

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
5	NA	A	603	-	-	-	X
7	EDO	A	614	-	-	-	X
7	EDO	B	511	-	-	-	X
7	EDO	B	512	-	-	X	-
7	EDO	B	515	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8966 atoms, of which 28 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	6	0
			4562	2949	762	843	8			

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	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	188	LEU	TYR	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

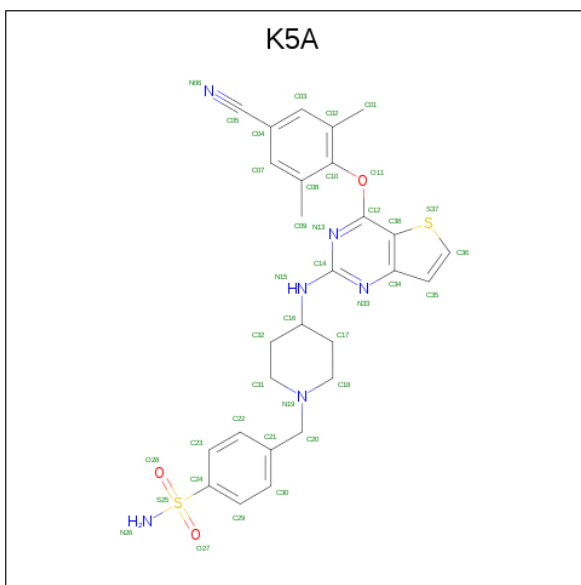
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	7	0
			3490	2276	575	632	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-cyano-2,6-dimethylphenoxy)thieno[3,2-d]pyrimidin-2-yl]amino}piperidin-1-yl)methyl]benzene-1-sulfonamide (three-letter code: K5A) (formula: C₂₇H₂₈N₆O₃S₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	
			66	27	28	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		
			1	1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na		
			1	1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

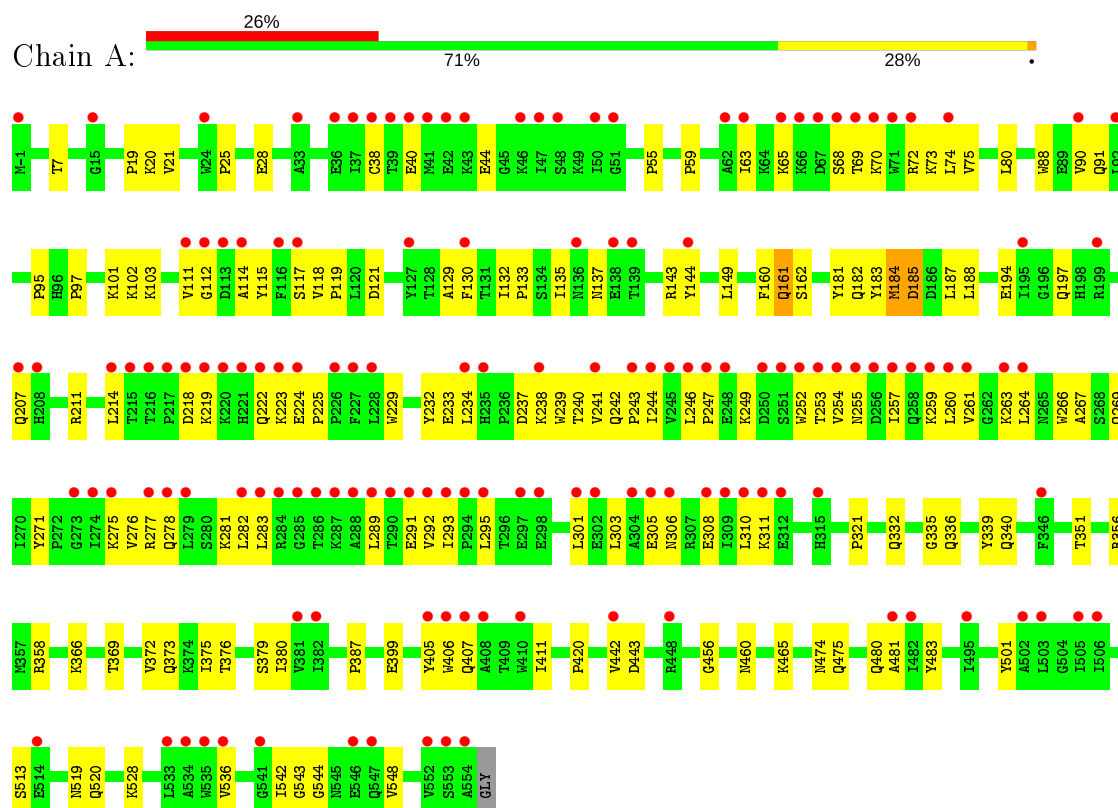
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	402	Total O 402 402	0	0
8	B	317	Total O 317 317	0	0

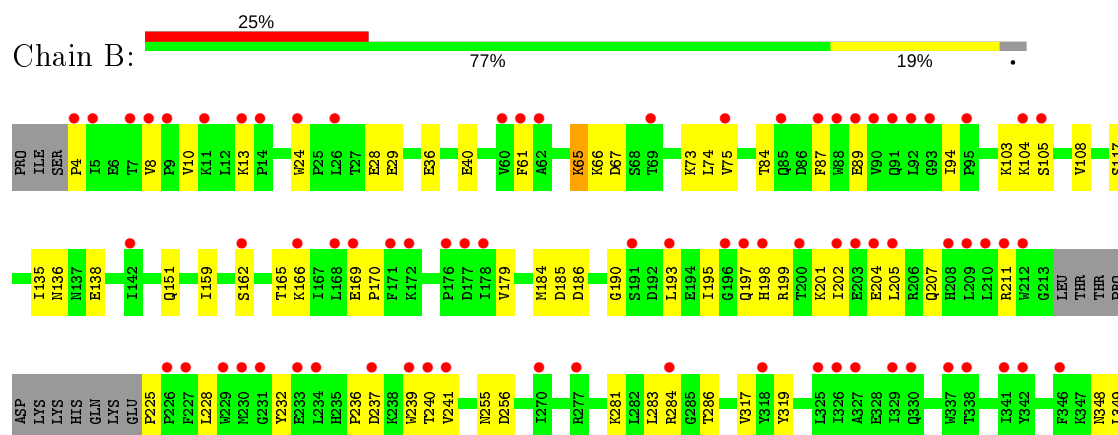
3 Residue-property plots

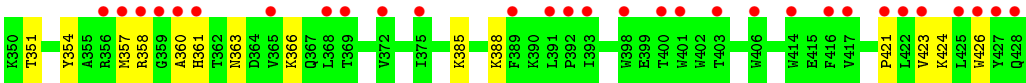
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: p51 RT





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.70Å 72.70Å 109.05Å 90.00° 100.21° 90.00°	Depositor
Resolution (Å)	42.06 – 1.94 42.07 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.06-1.94) 99.6 (42.07-1.94)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.194 , 0.232 0.196 , 0.233	Depositor DCC
R_{free} test set	4621 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.8	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	8966	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: NA, MG, EDO, K5A, 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	0.51	0/4680	0.49	0/6362
2	B	0.53	0/3594	0.52	0/4884
All	All	0.52	0/8274	0.50	0/11246

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	4562	0	4611	159	0
2	B	3490	0	3503	87	0
3	A	38	28	0	2	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	15	0	0	0	0
6	B	20	0	0	0	0
7	A	48	0	72	13	0
7	B	44	0	66	15	0
8	A	402	0	0	13	0
8	B	317	0	0	21	0
All	All	8938	28	8252	244	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 15.

All (244) 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:B:360:ALA:HB2	2:B:366:LYS:HD3	1.39	1.04
1:A:184:MET:HG2	1:A:185:ASP:H	1.25	1.00
1:A:399:GLU:HG2	7:A:614:EDO:H12	1.42	0.98
1:A:277:ARG:HB2	1:A:336[B]:GLN:HE21	1.25	0.97
1:A:259:LYS:HE2	1:A:263:LYS:HE3	1.43	0.97
1:A:544:GLY:HA2	2:B:286[B]:THR:HG22	1.47	0.95
2:B:255:ASN:HB3	7:B:512:EDO:H12	1.51	0.93
1:A:137:ASN:HB2	7:A:617:EDO:H22	1.56	0.88
1:A:277:ARG:HB2	1:A:336[B]:GLN:NE2	1.88	0.88
1:A:65:LYS:HE2	1:A:70:LYS:HE2	1.60	0.84
1:A:65:LYS:HE3	1:A:68:SER:HB3	1.58	0.83
1:A:246:LEU:HG	1:A:310:LEU:HD22	1.63	0.80
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.65	0.77
1:A:91:GLN:HB2	1:A:183:TYR:CE1	2.21	0.76
2:B:281:LYS:O	2:B:284:ARG:HG3	1.86	0.76
1:A:184:MET:CG	1:A:185:ASP:H	2.01	0.74
1:A:63:ILE:HD11	1:A:72:ARG:HB2	1.71	0.73
1:A:218:ASP:OD2	1:A:222:GLN:NE2	2.22	0.72
1:A:544:GLY:CA	2:B:286[B]:THR:HG22	2.19	0.72
2:B:256:ASP:OD1	7:B:512:EDO:H11	1.89	0.72
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.73	0.70
2:B:358:ARG:NH1	8:B:602:HOH:O	2.24	0.70
1:A:257:ILE:CG2	1:A:283:LEU:HD11	2.21	0.70
2:B:225:PRO:HB2	2:B:228:LEU:HB3	1.71	0.70
1:A:90:VAL:CG2	1:A:161:GLN:HG2	2.21	0.70
1:A:65:LYS:HG3	1:A:72:ARG:HH21	1.57	0.70
1:A:63:ILE:CD1	1:A:72:ARG:HB2	2.22	0.69
2:B:184:MET:HE3	8:B:740:HOH:O	1.91	0.69
1:A:88:TRP:CD1	1:A:90:VAL:HG12	2.27	0.69
1:A:260:LEU:O	1:A:264:LEU:HG	1.93	0.69
8:A:848:HOH:O	7:B:513:EDO:H21	1.92	0.69
1:A:336[B]:GLN:HA	1:A:336[B]:GLN:OE1	1.92	0.69
1:A:335:GLY:HA3	1:A:356[A]:ARG:HD3	1.75	0.69
2:B:65:LYS:NZ	8:B:603:HOH:O	2.25	0.68
2:B:135:ILE:HG21	7:B:513:EDO:H22	1.75	0.68
2:B:348:ASN:HB2	7:B:514:EDO:H11	1.76	0.67
2:B:162:SER:O	2:B:166:LYS:HD3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HG3	1:A:72:ARG:NH2	2.09	0.67
2:B:225:PRO:HG2	2:B:228:LEU:HD23	1.76	0.66
1:A:241:VAL:HG12	1:A:242:GLN:O	1.94	0.66
1:A:65:LYS:CE	1:A:70:LYS:HE2	2.25	0.66
1:A:183:TYR:O	1:A:184:MET:HB3	1.96	0.65
1:A:277:ARG:CB	1:A:336[B]:GLN:HE21	2.07	0.64
2:B:317:VAL:CG1	2:B:349:LEU:HD23	2.28	0.64
1:A:40:GLU:O	1:A:44:GLU:HG3	1.97	0.64
1:A:111:VAL:HG22	1:A:185:ASP:O	1.98	0.64
1:A:246:LEU:HG	1:A:310:LEU:CD2	2.28	0.63
2:B:162:SER:HB2	8:B:732:HOH:O	1.99	0.63
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.39	0.62
1:A:219:LYS:HE2	1:A:223:LYS:NZ	2.15	0.61
1:A:420:PRO:HG3	8:A:787:HOH:O	2.00	0.61
1:A:88:TRP:HD1	1:A:90:VAL:HG12	1.64	0.61
2:B:360:ALA:HB1	2:B:363:ASN:HB3	1.82	0.61
2:B:165:THR:O	2:B:169:GLU:HG2	2.00	0.60
2:B:198:HIS:O	2:B:202:ILE:HG12	2.01	0.60
1:A:88:TRP:CZ3	7:A:609:EDO:H11	2.37	0.60
1:A:162:SER:HB3	7:A:610:EDO:H11	1.84	0.60
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.84	0.59
1:A:399:GLU:CG	7:A:614:EDO:H12	2.26	0.59
2:B:255:ASN:CB	7:B:512:EDO:H12	2.28	0.59
2:B:184:MET:HE2	8:B:788:HOH:O	2.03	0.59
1:A:266:TRP:O	1:A:269:GLN:HG2	2.03	0.59
1:A:73:LYS:HB3	1:A:73:LYS:NZ	2.18	0.58
1:A:114:ALA:CB	1:A:214:LEU:HD22	2.33	0.58
1:A:184:MET:HG2	1:A:185:ASP:N	2.08	0.58
2:B:65:LYS:HD3	2:B:66:LYS:N	2.19	0.58
1:A:25:PRO:HA	8:A:881:HOH:O	2.04	0.58
1:A:369:THR:HG23	1:A:411:ILE:HD11	1.86	0.58
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.39	0.58
1:A:259:LYS:CE	1:A:263:LYS:HE3	2.26	0.57
1:A:73:LYS:HE2	1:A:75:VAL:HG23	1.86	0.57
1:A:306:ASN:O	1:A:310:LEU:HD13	2.06	0.56
2:B:284:ARG:HG2	8:B:753:HOH:O	2.04	0.56
2:B:207:GLN:O	2:B:211:ARG:N	2.35	0.56
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.86	0.56
7:A:610:EDO:H12	8:A:1042:HOH:O	2.04	0.56
1:A:257:ILE:O	1:A:261:VAL:HG23	2.06	0.55
1:A:253:THR:HG22	1:A:254:VAL:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TRP:HZ3	7:A:609:EDO:H11	1.69	0.55
7:B:511:EDO:H12	8:B:659:HOH:O	2.07	0.55
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.37	0.55
1:A:292:VAL:C	1:A:293:ILE:HD12	2.27	0.55
1:A:112:GLY:O	1:A:115:TYR:HB3	2.07	0.54
1:A:70:LYS:HE3	1:A:72:ARG:NE	2.22	0.54
1:A:475:GLN:HG3	7:A:611:EDO:O2	2.07	0.54
2:B:89:GLU:OE1	2:B:89:GLU:HA	2.08	0.54
1:A:90:VAL:HG21	1:A:161:GLN:HG2	1.89	0.54
1:A:513:SER:N	1:A:519:ASN:OD1	2.41	0.54
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.22	0.54
2:B:24:TRP:CD2	7:B:505:EDO:H21	2.42	0.54
2:B:40:GLU:HG2	8:B:691:HOH:O	2.08	0.54
1:A:65:LYS:HE2	1:A:70:LYS:CE	2.35	0.54
1:A:257:ILE:HG21	1:A:283:LEU:HD11	1.90	0.53
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.44	0.53
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.91	0.53
2:B:423:VAL:HA	2:B:426[B]:TRP:CD1	2.44	0.52
2:B:103:LYS:NZ	2:B:179:VAL:HG23	2.25	0.52
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.09	0.52
1:A:308:GLU:HA	1:A:311:LYS:HG3	1.91	0.52
2:B:195:ILE:HA	2:B:198:HIS:HB3	1.91	0.52
1:A:277:ARG:O	1:A:281:LYS:N	2.35	0.52
1:A:70:LYS:HE3	1:A:72:ARG:HG3	1.92	0.52
1:A:219:LYS:HE2	1:A:223:LYS:HZ1	1.75	0.52
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.09	0.52
1:A:528:LYS:HE2	7:A:608:EDO:H12	1.93	0.52
1:A:246:LEU:CG	1:A:310:LEU:HD22	2.39	0.51
2:B:105:SER:O	2:B:190:GLY:HA2	2.09	0.51
1:A:133:PRO:HB2	8:A:756:HOH:O	2.10	0.51
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.92	0.51
2:B:4:PRO:HG2	2:B:117:SER:O	2.11	0.51
1:A:253:THR:HG22	1:A:254:VAL:H	1.76	0.51
2:B:241:VAL:H	7:B:515:EDO:C2	2.22	0.51
1:A:188:LEU:N	1:A:188:LEU:HD12	2.26	0.51
1:A:254:VAL:HG23	1:A:291:GLU:O	2.11	0.51
1:A:233:GLU:OE2	1:A:243:PRO:HD3	2.11	0.50
1:A:254:VAL:HB	1:A:289:LEU:HA	1.93	0.50
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.93	0.50
1:A:261:VAL:HB	8:A:929:HOH:O	2.10	0.50
2:B:205:LEU:O	2:B:205:LEU:HD23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:O	1:A:282:LEU:HG	2.12	0.50
2:B:360:ALA:HB3	8:B:664:HOH:O	2.12	0.50
1:A:380[A]:ILE:HD11	7:B:509:EDO:H21	1.93	0.49
7:A:611:EDO:H21	8:A:919:HOH:O	2.12	0.49
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.46	0.49
2:B:197:GLN:O	2:B:201:LYS:HB2	2.12	0.49
1:A:283:LEU:N	1:A:283:LEU:HD12	2.28	0.49
2:B:193:LEU:HD13	2:B:197:GLN:HB2	1.95	0.49
2:B:225:PRO:HG2	2:B:228:LEU:CD2	2.41	0.49
1:A:239:TRP:O	1:A:240:THR:OG1	2.31	0.48
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.43	0.48
1:A:240:THR:HG22	1:A:241:VAL:N	2.28	0.48
1:A:91:GLN:HB2	1:A:183:TYR:HE1	1.72	0.48
2:B:236:PRO:HA	2:B:239:TRP:CG	2.49	0.48
1:A:118:VAL:HG11	1:A:149:LEU:HD11	1.96	0.48
1:A:267:ALA:HB1	1:A:271:TYR:CD2	2.49	0.48
2:B:66:LYS:O	2:B:67:ASP:HB2	2.13	0.48
1:A:244:ILE:HG22	1:A:310:LEU:HD23	1.96	0.48
2:B:8:VAL:O	2:B:10:VAL:HG23	2.13	0.48
2:B:207:GLN:HA	2:B:207:GLN:OE1	2.14	0.48
1:A:194:GLU:HG3	1:A:197:GLN:H	1.78	0.48
1:A:207:GLN:O	1:A:211:ARG:HD2	2.14	0.48
2:B:103:LYS:HD3	2:B:103:LYS:HA	1.56	0.48
1:A:376:THR:O	1:A:380[B]:ILE:HG12	2.13	0.48
1:A:460:ASN:HA	2:B:286[A]:THR:O	2.14	0.47
2:B:241:VAL:H	7:B:515:EDO:H22	1.77	0.47
1:A:443:ASP:HB2	1:A:548:VAL:HG13	1.96	0.47
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.79	0.47
2:B:13:LYS:HE3	2:B:84:THR:O	2.14	0.47
1:A:528:LYS:CE	7:A:608:EDO:H12	2.45	0.47
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.97	0.47
1:A:277:ARG:NH1	1:A:356[A]:ARG:HH11	2.12	0.46
1:A:480:GLN:HB2	8:A:948:HOH:O	2.14	0.46
2:B:8:VAL:HG21	2:B:159:ILE:HG23	1.97	0.46
1:A:358:ARG:NH1	8:A:724:HOH:O	2.48	0.46
1:A:237:ASP:O	1:A:238:LYS:HD3	2.16	0.46
1:A:244:ILE:HG22	1:A:310:LEU:CD2	2.46	0.46
1:A:111:VAL:HG22	1:A:185:ASP:C	2.37	0.46
1:A:456:GLY:HA3	1:A:465:LYS:O	2.16	0.46
2:B:421:PRO:HD2	8:B:696:HOH:O	2.16	0.46
2:B:65:LYS:HD3	2:B:66:LYS:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HE3	8:A:804:HOH:O	2.16	0.45
1:A:275:LYS:HG2	1:A:332:GLN:OE1	2.16	0.45
1:A:255:ASN:OD1	1:A:289:LEU:HD23	2.16	0.45
1:A:181:TYR:HB2	3:A:601:K5A:O11	2.16	0.45
1:A:95:PRO:HA	2:B:136:ASN:O	2.15	0.45
2:B:240:THR:HA	7:B:515:EDO:H21	1.98	0.45
1:A:257:ILE:HG22	1:A:283:LEU:HD11	1.98	0.45
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.52	0.45
2:B:186:ASP:HB2	8:B:624:HOH:O	2.15	0.45
2:B:255:ASN:OD1	7:B:512:EDO:H12	2.16	0.45
2:B:87:PHE:HB2	8:B:832:HOH:O	2.17	0.45
2:B:94:ILE:HD12	2:B:94:ILE:O	2.16	0.45
1:A:543:GLY:HA3	2:B:283:LEU:O	2.17	0.45
1:A:111:VAL:HG11	1:A:187:LEU:HG	1.99	0.45
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.52	0.45
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.99	0.45
1:A:115:TYR:HA	1:A:160:PHE:CE1	2.52	0.45
1:A:536:VAL:HB	1:A:542:ILE:HD13	1.99	0.45
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.47	0.45
2:B:28:GLU:HB2	2:B:135:ILE:HD11	2.00	0.45
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.52	0.45
1:A:240:THR:HG22	1:A:241:VAL:O	2.17	0.44
2:B:241:VAL:HG13	7:B:515:EDO:O2	2.17	0.44
1:A:184:MET:CG	1:A:185:ASP:N	2.72	0.44
3:A:601:K5A:C18	8:A:863:HOH:O	2.65	0.44
2:B:240:THR:HA	7:B:515:EDO:C2	2.48	0.44
2:B:10:VAL:HG13	2:B:87:PHE:HZ	1.83	0.44
1:A:162:SER:CB	7:A:610:EDO:H11	2.48	0.44
1:A:543:GLY:N	2:B:283:LEU:O	2.49	0.44
1:A:247:PRO:HB2	1:A:249:LYS:NZ	2.33	0.44
1:A:73:LYS:HG2	1:A:74:LEU:N	2.33	0.43
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.53	0.43
1:A:244:ILE:HA	8:A:839:HOH:O	2.18	0.43
1:A:69:THR:HG23	1:A:69:THR:O	2.17	0.43
1:A:102:LYS:O	1:A:103:LYS:HD3	2.18	0.43
2:B:241:VAL:HB	8:B:759:HOH:O	2.17	0.43
1:A:379:SER:CB	1:A:387:PRO:HD3	2.48	0.43
1:A:182:GLN:HB2	1:A:187:LEU:CD2	2.49	0.43
1:A:372:VAL:HG11	1:A:411:ILE:HD12	2.01	0.43
1:A:63:ILE:HD11	1:A:72:ARG:CB	2.45	0.43
2:B:225:PRO:HB2	2:B:228:LEU:CB	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:TYR:CD2	2:B:357:MET:HE1	2.53	0.43
1:A:474:ASN:HB2	7:A:611:EDO:H12	2.01	0.43
1:A:366:LYS:HE2	1:A:405:TYR:OH	2.19	0.42
1:A:243:PRO:HD2	8:A:956:HOH:O	2.19	0.42
1:A:129:ALA:HB1	1:A:143:ARG:NH2	2.35	0.42
1:A:406:TRP:CE2	1:A:407:GLN:HG3	2.55	0.42
2:B:36:GLU:HG3	8:B:711:HOH:O	2.18	0.42
1:A:114:ALA:HB1	1:A:214:LEU:HD13	2.01	0.42
1:A:7:THR:HG21	1:A:121:ASP:HA	2.02	0.42
1:A:91:GLN:HB2	1:A:183:TYR:CZ	2.55	0.42
1:A:117:SER:O	1:A:119:PRO:HD3	2.19	0.42
1:A:19:PRO:HD3	1:A:80:LEU:HD13	2.02	0.42
2:B:36:GLU:HG2	8:B:877:HOH:O	2.20	0.42
2:B:73:LYS:HZ3	2:B:75:VAL:CG2	2.32	0.42
2:B:104:LYS:HA	2:B:237:ASP:CG	2.40	0.42
2:B:199:ARG:O	8:B:601:HOH:O	2.22	0.42
2:B:29:GLU:HG2	8:B:607:HOH:O	2.20	0.42
1:A:101:LYS:HD3	1:A:321:PRO:CG	2.50	0.41
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.02	0.41
1:A:536:VAL:HB	1:A:542:ILE:CD1	2.51	0.41
2:B:136:ASN:HB3	2:B:138:GLU:HG3	2.02	0.41
1:A:219:LYS:HE2	1:A:223:LYS:HZ3	1.84	0.41
1:A:253:THR:HG22	1:A:289:LEU:O	2.20	0.41
2:B:361:HIS:HA	8:B:860:HOH:O	2.20	0.41
1:A:460:ASN:HA	2:B:286[B]:THR:O	2.20	0.41
1:A:267:ALA:HB1	1:A:271:TYR:HD2	1.84	0.41
1:A:369:THR:O	1:A:373:GLN:HG2	2.20	0.41
2:B:201:LYS:HA	2:B:201:LYS:HD2	1.84	0.41
1:A:339:TYR:CD2	1:A:375:ILE:HD11	2.56	0.41
2:B:351:THR:HG21	8:B:622:HOH:O	2.21	0.41
2:B:388:LYS:HE2	8:B:887:HOH:O	2.21	0.41
2:B:65:LYS:CD	2:B:66:LYS:H	2.34	0.41
1:A:369:THR:HA	1:A:411:ILE:HD11	2.03	0.41
2:B:228:LEU:O	2:B:228:LEU:HD12	2.21	0.41
2:B:424:LYS:HE3	8:B:685:HOH:O	2.20	0.41
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.56	0.40
1:A:513:SER:O	1:A:519:ASN:ND2	2.48	0.40
1:A:224:GLU:HB3	1:A:225:PRO:HD2	2.04	0.40
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.56	0.40
1:A:246:LEU:HD22	1:A:260:LEU:HD11	2.04	0.40
1:A:411:ILE:HA	1:A:411:ILE:HD13	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:HD13	1:A:306:ASN:ND2	2.37	0.40
1:A:301:LEU:O	1:A:305:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	560/557 (100%)	541 (97%)	17 (3%)	2 (0%)	34	24
2	B	417/428 (97%)	396 (95%)	21 (5%)	0	100	100
All	All	977/985 (99%)	937 (96%)	38 (4%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	MET
1	A	276	VAL

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	500/495 (101%)	498 (100%)	2 (0%)	91	91
2	B	383/390 (98%)	381 (100%)	2 (0%)	88	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	883/885 (100%)	879 (100%)	4 (0%)	88	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	185	ASP
2	B	65	LYS
2	B	204	GLU

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

Mol	Chain	Res	Type
1	A	161	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 2 are monoatomic - leaving 31 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	K5A	A	601	-	40,42,42	2.40	11 (27%)	50,61,61	2.83	22 (44%)
6	SO4	A	605	-	4,4,4	0.16	0	6,6,6	0.09	0
7	EDO	A	614	-	3,3,3	0.42	0	2,2,2	0.33	0
7	EDO	A	611	-	3,3,3	0.46	0	2,2,2	0.42	0
7	EDO	A	618	-	3,3,3	0.45	0	2,2,2	0.34	0
6	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.04	0
7	EDO	A	615	-	3,3,3	0.46	0	2,2,2	0.35	0
6	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	B	504	-	4,4,4	0.13	0	6,6,6	0.06	0
7	EDO	B	510	-	3,3,3	0.42	0	2,2,2	0.32	0
7	EDO	A	612	-	3,3,3	0.44	0	2,2,2	0.39	0
7	EDO	A	617	-	3,3,3	0.41	0	2,2,2	0.34	0
7	EDO	A	616	-	3,3,3	0.52	0	2,2,2	0.36	0
7	EDO	B	512	-	3,3,3	0.37	0	2,2,2	0.34	0
7	EDO	B	511	-	3,3,3	0.49	0	2,2,2	0.41	0
7	EDO	B	509	-	3,3,3	0.48	0	2,2,2	0.44	0
6	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.06	0
7	EDO	B	513	-	3,3,3	0.41	0	2,2,2	0.35	0
7	EDO	A	607	-	3,3,3	0.43	0	2,2,2	0.42	0
7	EDO	A	610	-	3,3,3	0.45	0	2,2,2	0.33	0
7	EDO	B	515	-	3,3,3	0.43	0	2,2,2	0.34	0
6	SO4	A	606	-	4,4,4	0.12	0	6,6,6	0.05	0
7	EDO	B	507	-	3,3,3	0.49	0	2,2,2	0.31	0
7	EDO	A	608	-	3,3,3	0.40	0	2,2,2	0.35	0
7	EDO	B	514	-	3,3,3	0.45	0	2,2,2	0.31	0
7	EDO	A	609	-	3,3,3	0.50	0	2,2,2	0.28	0
7	EDO	A	613	-	3,3,3	0.46	0	2,2,2	0.36	0
7	EDO	B	505	-	3,3,3	0.33	0	2,2,2	0.29	0
6	SO4	A	604	-	4,4,4	0.16	0	6,6,6	0.07	0
7	EDO	B	508	-	3,3,3	0.47	0	2,2,2	0.45	0
7	EDO	B	506	-	3,3,3	0.37	0	2,2,2	0.14	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	K5A	A	601	-	-	1/20/30/30	0/5/5/5
7	EDO	A	614	-	-	0/1/1/1	-
7	EDO	A	611	-	-	0/1/1/1	-
7	EDO	A	618	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	615	-	-	0/1/1/1	-
7	EDO	A	613	-	-	0/1/1/1	-
7	EDO	B	510	-	-	0/1/1/1	-
7	EDO	A	612	-	-	0/1/1/1	-
7	EDO	A	617	-	-	0/1/1/1	-
7	EDO	A	616	-	-	1/1/1/1	-
7	EDO	B	512	-	-	0/1/1/1	-
7	EDO	B	511	-	-	0/1/1/1	-
7	EDO	B	509	-	-	0/1/1/1	-
7	EDO	B	513	-	-	0/1/1/1	-
7	EDO	A	607	-	-	0/1/1/1	-
7	EDO	A	610	-	-	0/1/1/1	-
7	EDO	B	515	-	-	0/1/1/1	-
7	EDO	B	507	-	-	0/1/1/1	-
7	EDO	A	608	-	-	0/1/1/1	-
7	EDO	B	514	-	-	0/1/1/1	-
7	EDO	A	609	-	-	0/1/1/1	-
7	EDO	B	505	-	-	0/1/1/1	-
7	EDO	B	508	-	-	0/1/1/1	-
7	EDO	B	506	-	-	1/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	K5A	S25-N26	7.47	1.75	1.60
3	A	601	K5A	C18-N19	6.74	1.65	1.46
3	A	601	K5A	C14-N15	5.47	1.41	1.34
3	A	601	K5A	C32-C16	4.72	1.63	1.52
3	A	601	K5A	C12-N13	3.65	1.38	1.31
3	A	601	K5A	C14-N13	3.04	1.44	1.34
3	A	601	K5A	C17-C16	2.91	1.58	1.52
3	A	601	K5A	C10-C08	2.36	1.44	1.40
3	A	601	K5A	C29-C24	2.25	1.42	1.38
3	A	601	K5A	C16-N15	2.24	1.51	1.46
3	A	601	K5A	O11-C12	2.01	1.39	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	K5A	C03-C04-C05	6.58	128.28	119.54
3	A	601	K5A	C20-N19-C31	6.37	125.24	111.06
3	A	601	K5A	C21-C20-N19	-5.54	102.38	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	K5A	C29-C24-C23	-5.36	112.96	120.44
3	A	601	K5A	C07-C04-C05	-5.12	112.74	119.54
3	A	601	K5A	C22-C23-C24	4.88	124.50	119.45
3	A	601	K5A	C17-C18-N19	4.71	118.42	111.11
3	A	601	K5A	C01-C02-C10	4.54	128.15	120.82
3	A	601	K5A	C30-C29-C24	4.13	123.72	119.45
3	A	601	K5A	C31-N19-C18	4.08	118.01	108.83
3	A	601	K5A	C01-C02-C03	-3.93	112.22	119.49
3	A	601	K5A	O11-C12-C38	3.38	121.19	115.69
3	A	601	K5A	C17-C16-N15	3.35	115.81	110.60
3	A	601	K5A	C23-C24-S25	3.21	124.39	119.73
3	A	601	K5A	C32-C31-N19	2.79	115.44	111.11
3	A	601	K5A	C32-C16-C17	-2.77	106.02	110.82
3	A	601	K5A	C09-C08-C10	2.76	125.27	120.82
3	A	601	K5A	O28-S25-N26	2.70	111.37	107.36
3	A	601	K5A	C18-C17-C16	2.62	115.10	110.50
3	A	601	K5A	O28-S25-O27	-2.56	114.56	118.76
3	A	601	K5A	N15-C14-N13	2.26	120.57	117.18
3	A	601	K5A	C29-C24-S25	2.00	122.64	119.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	K5A	C21-C20-N19-C18
7	A	616	EDO	O1-C1-C2-O2
7	B	506	EDO	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 30 short contacts:

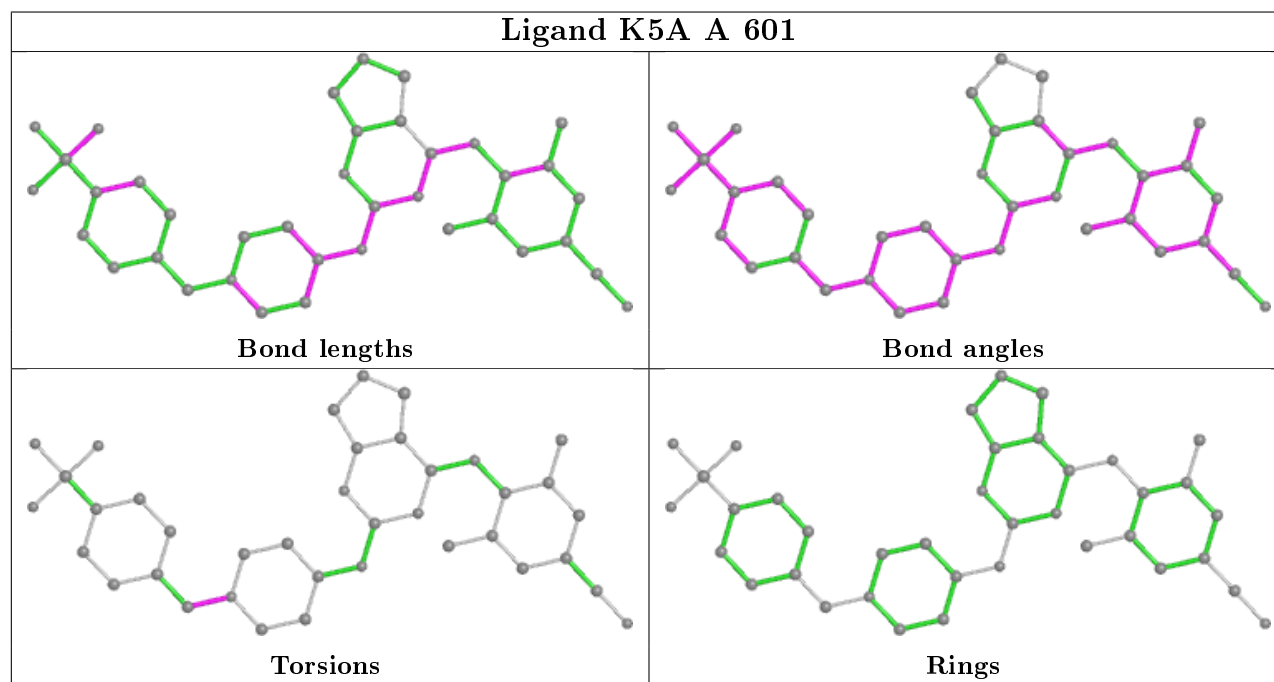
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	K5A	2	0
7	A	614	EDO	2	0
7	A	611	EDO	3	0
7	A	617	EDO	1	0
7	B	512	EDO	4	0
7	B	511	EDO	1	0
7	B	509	EDO	1	0
7	B	513	EDO	2	0
7	A	610	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	515	EDO	5	0
7	A	608	EDO	2	0
7	B	514	EDO	1	0
7	A	609	EDO	2	0
7	B	505	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 ⓘ

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	556/557 (99%)	1.53	145 (26%) 0 0	41, 80, 173, 253	0
2	B	414/428 (96%)	1.42	106 (25%) 0 0	42, 70, 140, 287	0
All	All	970/985 (98%)	1.48	251 (25%) 0 0	41, 75, 162, 287	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	ILE	20.6
1	A	286	THR	16.2
1	A	221	HIS	13.8
1	A	292	VAL	13.0
2	B	4	PRO	13.0
2	B	90	VAL	12.9
2	B	91	GLN	12.9
1	A	67	ASP	11.8
2	B	92	LEU	10.4
1	A	220	LYS	9.8
1	A	261	VAL	9.7
1	A	290	THR	9.7
2	B	89	GLU	9.2
1	A	283	LEU	9.1
1	A	252	TRP	8.9
1	A	68	SER	8.5
1	A	254	VAL	8.4
1	A	244	ILE	8.2
1	A	227	PHE	7.4
1	A	309	ILE	7.4
1	A	295	LEU	7.2
1	A	301	LEU	7.2
1	A	282	LEU	7.1
1	A	218	ASP	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	6.9
1	A	260	LEU	6.8
2	B	210	LEU	6.7
2	B	5	ILE	6.6
1	A	293	ILE	6.6
1	A	289	LEU	6.6
1	A	72	ARG	6.4
1	A	284	ARG	6.4
2	B	359	GLY	6.3
1	A	245	VAL	6.3
1	A	222	GLN	6.3
1	A	66	LYS	6.1
2	B	226	PRO	6.0
1	A	223	LYS	6.0
1	A	304	ALA	5.9
2	B	209	LEU	5.8
2	B	358	ARG	5.6
1	A	256	ASP	5.6
1	A	138	GLU	5.5
1	A	273	GLY	5.5
1	A	219	LYS	5.5
1	A	63	ILE	5.5
2	B	230	MET	5.4
1	A	294	PRO	5.4
1	A	24	TRP	5.4
1	A	215	THR	5.4
1	A	288	ALA	5.4
2	B	193	LEU	5.3
2	B	88	TRP	5.2
1	A	278	GLN	5.2
1	A	546	GLU	5.1
1	A	255	ASN	4.9
1	A	217	PRO	4.9
1	A	297	GLU	4.9
1	A	114	ALA	4.8
2	B	357	MET	4.8
1	A	250	ASP	4.7
2	B	227	PHE	4.7
2	B	427[A]	TYR	4.7
2	B	166	LYS	4.6
2	B	229	TRP	4.6
2	B	204	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	116	PHE	4.5
1	A	274	ILE	4.5
2	B	14	PRO	4.5
1	A	287	LYS	4.5
1	A	195	ILE	4.5
2	B	202	ILE	4.5
1	A	406	TRP	4.4
1	A	90	VAL	4.4
2	B	372	VAL	4.4
1	A	74	LEU	4.4
2	B	422	LEU	4.4
1	A	311	LYS	4.4
2	B	104	LYS	4.4
2	B	200	THR	4.3
1	A	199	ARG	4.3
1	A	298	GLU	4.3
1	A	71	TRP	4.3
2	B	391	LEU	4.2
1	A	139	THR	4.1
1	A	50	ILE	4.1
1	A	291	GLU	4.1
2	B	212	TRP	4.1
2	B	368	LEU	4.1
2	B	393	ILE	4.0
2	B	105	SER	4.0
1	A	247	PRO	4.0
2	B	197	GLN	4.0
2	B	365	VAL	4.0
1	A	144	TYR	3.9
2	B	87	PHE	3.8
1	A	136	ASN	3.8
2	B	233	GLU	3.8
1	A	275	LYS	3.8
2	B	205	LEU	3.8
1	A	111	VAL	3.8
2	B	231	GLY	3.7
2	B	326	ILE	3.7
2	B	240	THR	3.7
1	A	37	ILE	3.7
2	B	8	VAL	3.7
1	A	285	GLY	3.7
1	A	554	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	482	ILE	3.6
1	A	251	SER	3.6
2	B	7	THR	3.6
2	B	270	ILE	3.6
1	A	92	LEU	3.6
1	A	302	GLU	3.6
2	B	337	TRP	3.5
2	B	93	GLY	3.5
1	A	503	LEU	3.5
1	A	552	VAL	3.5
1	A	279	LEU	3.5
1	A	533	LEU	3.5
1	A	224	GLU	3.4
1	A	241	VAL	3.4
2	B	414	TRP	3.4
1	A	65	LYS	3.3
1	A	410	TRP	3.3
2	B	169	GLU	3.3
2	B	398	TRP	3.3
2	B	425	LEU	3.3
2	B	60[A]	VAL	3.2
2	B	392	PRO	3.2
2	B	426[A]	TRP	3.2
1	A	33	ALA	3.2
2	B	168	LEU	3.2
1	A	38	CYS	3.2
2	B	338	THR	3.1
2	B	191	SER	3.1
1	A	70	LYS	3.1
1	A	15	GLY	3.1
1	A	234	LEU	3.1
2	B	172	LYS	3.1
2	B	284	ARG	3.1
2	B	75	VAL	3.1
1	A	506	ILE	3.1
1	A	253	THR	3.1
1	A	36	GLU	3.0
1	A	226	PRO	3.0
1	A	117	SER	3.0
1	A	277	ARG	3.0
2	B	361	HIS	3.0
1	A	214	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	95	PRO	3.0
2	B	421	PRO	3.0
1	A	40	GLU	3.0
1	A	216	THR	3.0
1	A	310	LEU	3.0
2	B	356	ARG	3.0
1	A	259	LYS	2.9
2	B	13	LYS	2.9
2	B	360	ALA	2.9
2	B	329	ILE	2.9
1	A	62	ALA	2.9
1	A	243	PRO	2.9
2	B	428	GLN	2.8
2	B	423	VAL	2.8
1	A	228	LEU	2.8
1	A	263	LYS	2.8
1	A	47	ILE	2.8
1	A	408	ALA	2.8
2	B	375	ILE	2.8
1	A	306	ASN	2.8
2	B	239	TRP	2.8
2	B	198	HIS	2.8
2	B	234	LEU	2.8
2	B	403	THR	2.8
2	B	318	TYR	2.8
1	A	541	GLY	2.7
1	A	312	GLU	2.7
1	A	235	HIS	2.7
2	B	26	LEU	2.7
1	A	382	ILE	2.6
1	A	502	ALA	2.6
1	A	505	ILE	2.6
1	A	-1	MET	2.6
1	A	315[A]	HIS	2.6
1	A	43	LYS	2.6
2	B	346	PHE	2.6
1	A	246	LEU	2.6
1	A	208	HIS	2.6
2	B	241	VAL	2.6
1	A	41	MET	2.6
1	A	481	ALA	2.5
2	B	11	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	24	TRP	2.5
2	B	342	TYR	2.5
1	A	264	LEU	2.5
1	A	407	GLN	2.5
2	B	208	HIS	2.5
2	B	277	ARG	2.5
2	B	369	THR	2.5
2	B	196	GLY	2.4
2	B	69	THR	2.4
1	A	346	PHE	2.4
2	B	416	PHE	2.4
2	B	417	VAL	2.4
1	A	547	GLN	2.4
1	A	207	GLN	2.4
1	A	553	SER	2.4
2	B	203	GLU	2.4
2	B	327	ALA	2.4
1	A	305	GLU	2.4
1	A	495	ILE	2.4
1	A	127	TYR	2.3
1	A	238	LYS	2.3
1	A	42	GLU	2.3
1	A	48	SER	2.3
1	A	448	ARG	2.3
2	B	171	PHE	2.3
1	A	113	ASP	2.3
2	B	9	PRO	2.3
1	A	308	GLU	2.2
2	B	176	PRO	2.2
1	A	536	VAL	2.2
2	B	341	ILE	2.2
1	A	51	GLY	2.2
2	B	325	LEU	2.2
2	B	401	TRP	2.2
2	B	85	GLN	2.2
1	A	535	TRP	2.2
1	A	514	GLU	2.2
2	B	178	ILE	2.1
1	A	248	GLU	2.1
2	B	400	THR	2.1
2	B	330	GLN	2.1
1	A	130	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	112	GLY	2.1
2	B	237	ASP	2.1
1	A	46	LYS	2.1
1	A	405	TYR	2.1
1	A	381	VAL	2.1
1	A	534	ALA	2.1
2	B	211	ARG	2.1
1	A	442	VAL	2.1
2	B	61	PHE	2.1
2	B	389	PHE	2.1
2	B	62	ALA	2.0
2	B	177	ASP	2.0
1	A	39	THR	2.0
2	B	406	TRP	2.0
1	A	258	GLN	2.0
2	B	142	ILE	2.0
2	B	162	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.

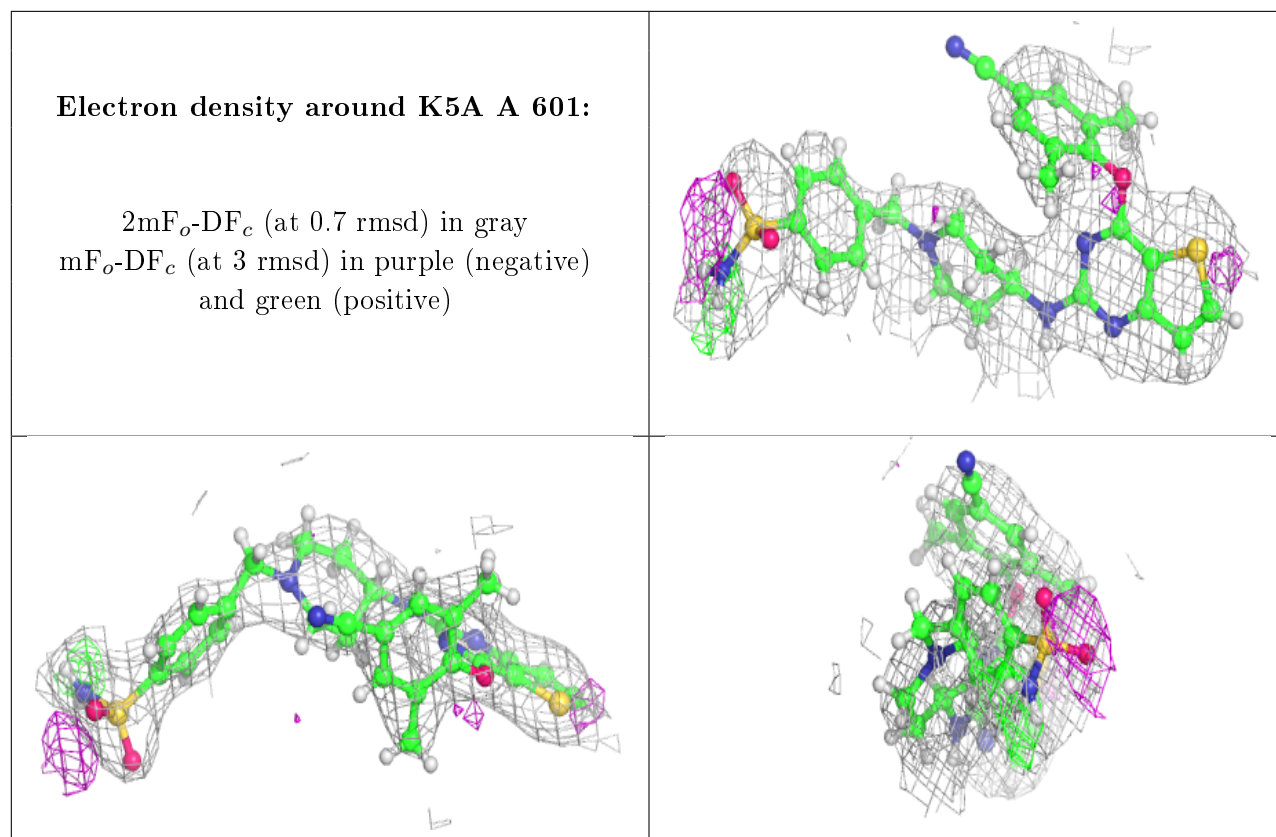
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	A	616	4/4	0.50	0.32	88,89,91,94	0
7	EDO	B	515	4/4	0.58	0.20	121,123,125,125	0
7	EDO	A	609	4/4	0.60	0.34	98,99,100,101	0
7	EDO	A	610	4/4	0.62	0.40	109,112,116,118	0
5	NA	A	603	1/1	0.65	0.66	125,125,125,125	0
6	SO4	B	501	5/5	0.70	0.28	211,211,211,211	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	614	4/4	0.73	0.41	97,102,108,111	0
6	SO4	A	606	5/5	0.76	0.18	148,148,149,151	0
7	EDO	A	611	4/4	0.76	0.13	76,79,81,85	0
7	EDO	B	513	4/4	0.77	0.29	93,96,96,96	0
7	EDO	B	511	4/4	0.78	0.51	83,85,87,88	0
7	EDO	A	613	4/4	0.78	0.27	106,107,107,109	0
7	EDO	B	507	4/4	0.78	0.20	93,94,96,98	0
7	EDO	A	615	4/4	0.78	0.23	92,93,97,100	0
7	EDO	B	508	4/4	0.80	0.20	85,87,88,91	0
7	EDO	B	509	4/4	0.81	0.34	73,75,78,83	0
7	EDO	B	510	4/4	0.81	0.19	83,89,96,100	0
6	SO4	B	504	5/5	0.82	0.24	156,156,157,157	0
7	EDO	A	617	4/4	0.82	0.60	109,110,111,113	0
7	EDO	A	612	4/4	0.85	0.19	94,95,95,97	0
7	EDO	B	514	4/4	0.86	0.51	132,132,133,133	0
4	MG	A	602	1/1	0.88	0.28	67,67,67,67	0
7	EDO	B	512	4/4	0.88	0.37	99,100,100,101	0
6	SO4	A	604	5/5	0.89	0.27	115,116,118,121	0
6	SO4	B	503	5/5	0.90	0.20	143,144,144,144	0
6	SO4	B	502	5/5	0.90	0.28	147,148,149,149	0
7	EDO	A	607	4/4	0.90	0.18	60,65,69,77	0
3	K5A	A	601	38/38	0.90	0.16	57,100,145,153	0
7	EDO	A	608	4/4	0.90	0.22	79,81,86,88	0
7	EDO	B	506	4/4	0.92	0.22	66,67,67,69	0
6	SO4	A	605	5/5	0.94	0.10	110,113,115,119	0
7	EDO	A	618	4/4	0.94	0.32	31,34,39,43	0
7	EDO	B	505	4/4	0.95	0.31	55,61,62,67	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.