



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:54 PM UTC

PDB ID : 6HXF / pdb_00006hxf
Title : Human STK10 bound to a maleimide inhibitor
Authors : Sorrell, F.J.; Salah, E.; Serafim, R.A.M.; Savitsky, P.A.; Krojer, T.; Bailey, H.J.; Pinkas, D.; Burgess-Brown, N.A.; von Delft, F.; Knapp, S.; Arrowsmith, C.; Bountra, C.; Edwards, A.M.; Elkins, J.M.
Deposited on : 2018-10-17
Resolution : 2.09 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

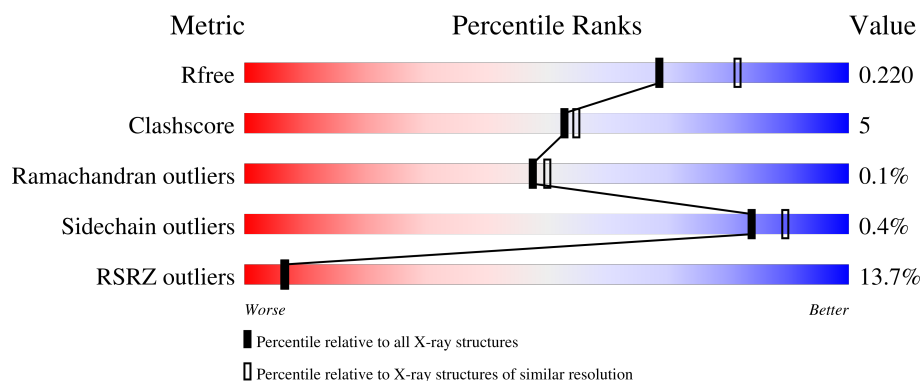
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	302	16% 84% 10% 6%
1	B	302	14% 85% 10% . .
1	C	302	14% 83% 12% . 5%
1	D	302	8% 86% 8% . 5%

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
1	SEP	C	191	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9913 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.

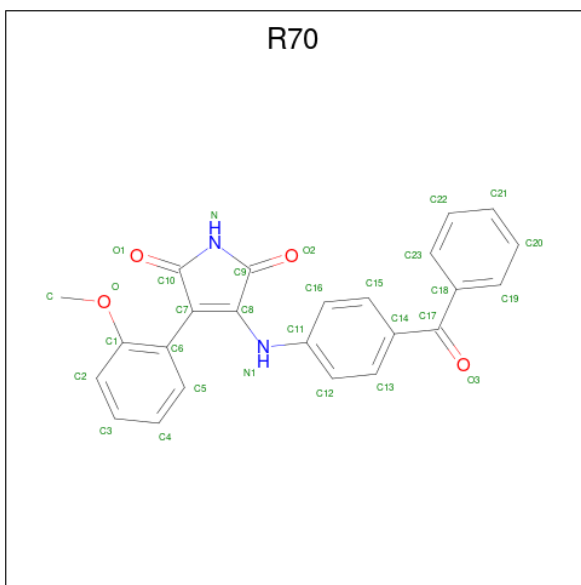
- Molecule 1 is a protein called Serine/threonine-protein kinase 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	291	Total	C	N	O	P	S	0	9	0
			2280	1463	373	425	3	16			
1	A	285	Total	C	N	O	P	S	0	5	0
			2184	1402	355	409	3	15			
1	C	288	Total	C	N	O	P	S	0	10	0
			2289	1471	377	420	3	18			
1	D	287	Total	C	N	O	P	S	0	10	0
			2282	1474	369	423	2	14			

There are 8 discrepancies between the modelled and reference sequences:

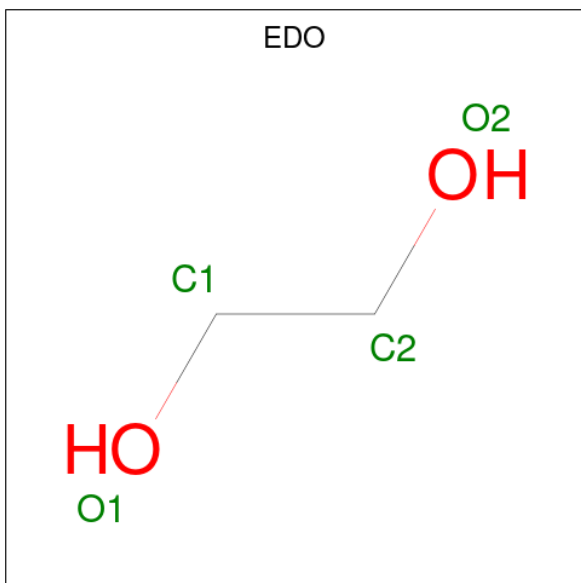
Chain	Residue	Modelled	Actual	Comment	Reference
B	16	SER	-	expression tag	UNP O94804
B	17	MET	-	expression tag	UNP O94804
A	16	SER	-	expression tag	UNP O94804
A	17	MET	-	expression tag	UNP O94804
C	16	SER	-	expression tag	UNP O94804
C	17	MET	-	expression tag	UNP O94804
D	16	SER	-	expression tag	UNP O94804
D	17	MET	-	expression tag	UNP O94804

- Molecule 2 is 3-(2-methoxyphenyl)-4-[[4-(phenylcarbonyl)phenyl]amino]pyrrole-2,5-dione (CCD ID: R70) (formula: C₂₄H₁₈N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			30	24	2	4		
2	A	1	Total	C	N	O	0	0
			30	24	2	4		
2	C	1	Total	C	N	O	0	0
			30	24	2	4		
2	D	1	Total	C	N	O	0	0
			30	24	2	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

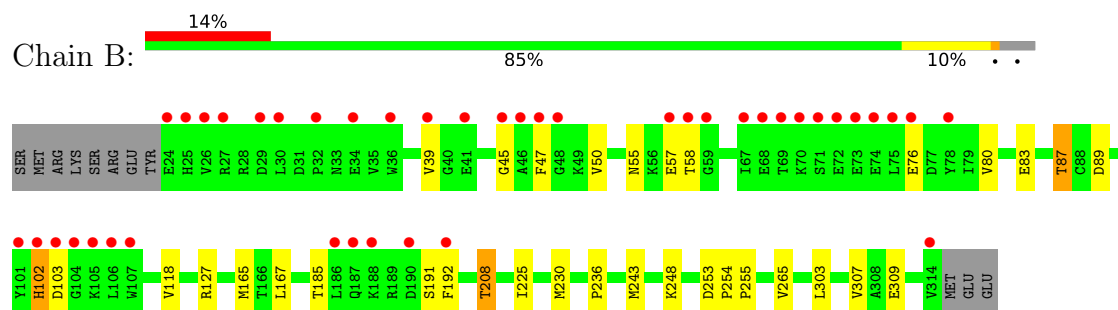
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	203	Total O 203 203	0	0
5	A	158	Total O 158 158	0	0
5	C	176	Total O 176 176	0	0
5	D	188	Total O 188 188	0	0

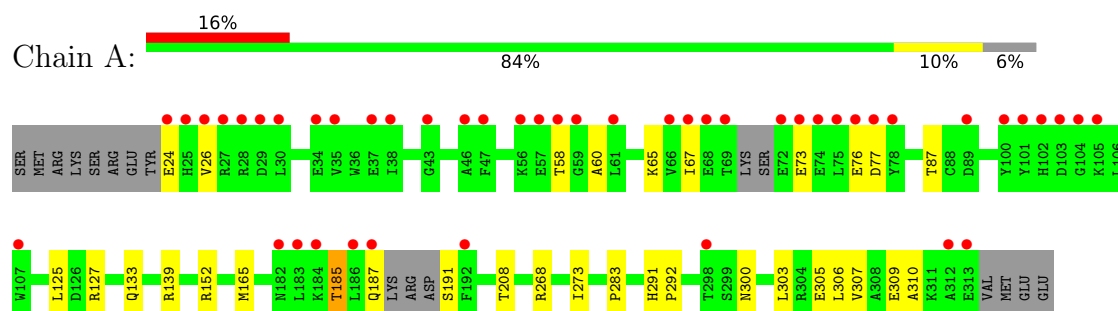
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

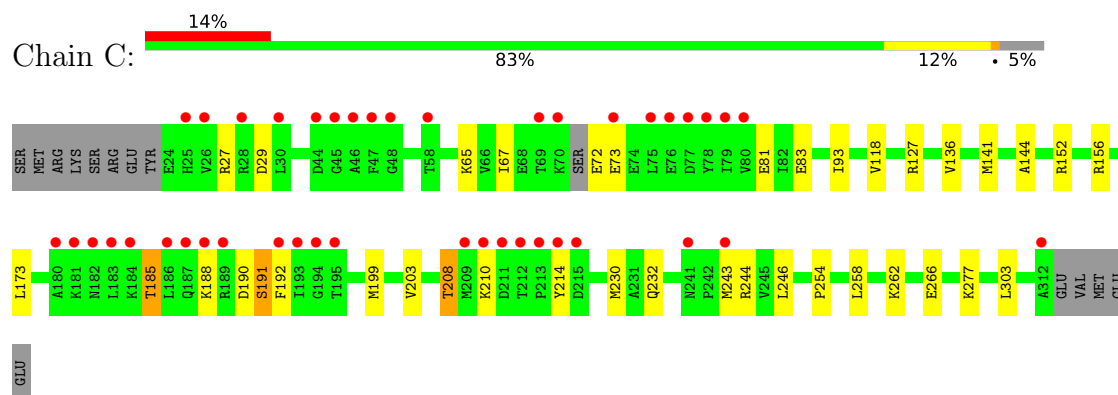
• Molecule 1: Serine/threonine-protein kinase 10



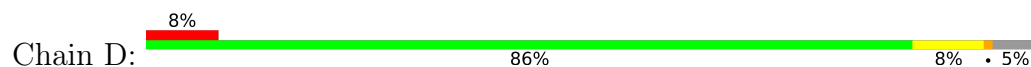
• Molecule 1: Serine/threonine-protein kinase 10

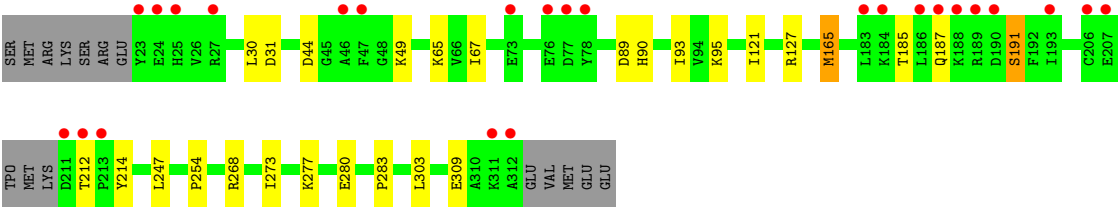


• Molecule 1: Serine/threonine-protein kinase 10



• Molecule 1: Serine/threonine-protein kinase 10





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.84Å 101.67Å 198.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.45 – 2.09 65.45 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.45-2.09) 100.0 (65.45-2.09)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.08Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.190 , 0.219 0.192 , 0.220	Depositor DCC
R_{free} test set	5503 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9913	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3446e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R70, SEP, EDO, TPO, CL

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	0.44	0/2210	0.55	0/3007
1	B	0.50	0/2318	0.70	4/3148 (0.1%)
1	C	0.47	0/2327	0.67	1/3153 (0.0%)
1	D	0.50	0/2338	0.59	0/3174
All	All	0.48	0/9193	0.63	5/12482 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	VAL	CG1-CB-CG2	6.40	124.89	110.80
1	B	58	THR	OG1-CB-CG2	6.35	122.00	109.30
1	C	83	GLU	CA-CB-CG	5.83	125.76	114.10
1	B	102	HIS	N-CA-CB	5.82	120.93	111.21
1	B	58	THR	CA-CB-CG2	5.18	119.31	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2184	0	2120	23	0
1	B	2280	0	2241	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2289	0	2277	28	0
1	D	2282	0	2283	20	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0
3	B	16	0	24	0	0
3	C	4	0	6	0	0
3	D	12	0	18	0	0
4	A	1	0	0	0	0
5	A	158	0	0	4	2
5	B	203	0	0	6	0
5	C	176	0	0	8	1
5	D	188	0	0	6	1
All	All	9913	0	8969	91	2

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 5.

All (91) 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:C:244:ARG:NH1	5:C:502:HOH:O	1.98	0.96
1:C:127:ARG:NH2	5:C:503:HOH:O	2.03	0.91
1:D:30:LEU:O	5:D:501:HOH:O	1.93	0.85
1:D:268:ARG:HD2	5:D:502:HOH:O	1.83	0.78
1:D:165[B]:MET:HE1	1:D:303:LEU:HD13	1.67	0.77
1:B:253:ASP:OD2	5:B:501:HOH:O	2.04	0.76
1:A:76:GLU:HG3	1:A:77:ASP:N	2.05	0.70
1:C:208:TPO:O1P	5:C:504:HOH:O	2.10	0.68
1:C:232:GLN:HE22	1:C:258:LEU:HD23	1.59	0.68
1:A:65:LYS:HE2	1:A:67:ILE:HD11	1.75	0.68
1:C:232:GLN:NE2	1:C:258:LEU:HD23	2.11	0.66
1:B:83:GLU:OE1	5:B:502:HOH:O	2.13	0.65
1:C:188:LYS:NZ	5:C:501:HOH:O	1.95	0.65
1:C:266:GLU:OE2	5:C:505:HOH:O	2.15	0.64
1:C:203:VAL:HG22	1:C:214:TYR:CG	2.35	0.61
1:B:208:TPO:O1P	5:B:503:HOH:O	2.17	0.60
1:C:262:LYS:HE3	5:C:655:HOH:O	2.00	0.60
1:A:185:TPO:HG22	1:A:187:GLN:H	1.68	0.58
1:A:268:ARG:HD2	5:A:504:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:PRO:HG3	1:C:277:LYS:HG3	1.84	0.58
1:A:76:GLU:HG3	1:A:77:ASP:H	1.67	0.58
1:A:152:ARG:HD3	5:A:631:HOH:O	2.04	0.57
1:C:192:PHE:CE2	1:C:199[A]:MET:HE1	2.39	0.57
1:B:127:ARG:HH22	1:B:309:GLU:CD	2.13	0.56
1:A:165[B]:MET:HE1	1:A:303:LEU:HD22	1.88	0.56
1:D:187:GLN:NE2	5:D:504:HOH:O	2.39	0.56
1:B:102:HIS:ND1	1:B:103:ASP:N	2.54	0.56
1:A:24:GLU:HG2	1:A:26:VAL:H	1.70	0.56
1:A:58:THR:HG23	1:A:60:ALA:H	1.71	0.55
1:A:87:THR:HG21	5:D:627:HOH:O	2.06	0.55
1:A:303:LEU:O	1:A:307:VAL:HG23	2.07	0.55
1:D:214:TYR:CE2	1:D:280:GLU:HG2	2.42	0.54
1:A:165[A]:MET:HE1	1:A:303:LEU:HD13	1.89	0.54
1:C:156:ARG:NH1	1:C:191:SEP:O1P	2.41	0.54
1:B:243[B]:MET:HA	1:C:243[B]:MET:HE2	1.90	0.53
1:D:127[A]:ARG:NH2	1:D:309:GLU:OE2	2.41	0.53
1:B:165[B]:MET:HE3	1:B:303:LEU:HD13	1.90	0.52
1:C:65:LYS:HE2	1:C:67:ILE:HD11	1.91	0.52
1:B:102:HIS:CG	1:B:103:ASP:H	2.27	0.51
1:D:30:LEU:HD12	1:D:31:ASP:N	2.26	0.51
1:C:152:ARG:HD2	1:C:185:TPO:HA	1.92	0.51
1:D:30:LEU:HD12	1:D:31:ASP:H	1.76	0.50
1:D:90:HIS:HB3	1:D:93[A]:ILE:HD12	1.94	0.50
1:D:254:PRO:HG3	1:D:277:LYS:HG3	1.93	0.49
1:C:141[B]:MET:SD	1:C:173:LEU:HD21	2.53	0.48
1:A:127:ARG:NH2	5:A:510:HOH:O	2.39	0.48
1:C:246:LEU:HD22	1:C:246:LEU:H	1.78	0.48
1:B:76:GLU:O	1:B:80:VAL:HG23	2.15	0.47
1:A:133:GLN:NE2	1:A:306:LEU:HB2	2.29	0.47
1:B:47:PHE:HE2	1:B:50:VAL:HG23	1.79	0.47
1:A:125:LEU:HD21	1:A:310:ALA:HA	1.97	0.47
1:D:65:LYS:HE2	1:D:67:ILE:HD11	1.97	0.47
1:A:87:THR:CG2	5:D:507:HOH:O	2.63	0.46
1:D:121:ILE:HD12	1:D:165[A]:MET:CE	2.45	0.46
1:D:165[B]:MET:CE	1:D:303:LEU:HD13	2.43	0.46
1:D:187:GLN:HG3	1:D:191:SEP:HB2	1.98	0.46
1:B:265[A]:VAL:HG23	5:B:634:HOH:O	2.15	0.46
1:D:303:LEU:HD23	1:D:303:LEU:HA	1.74	0.46
1:B:89:ASP:OD2	1:B:89:ASP:N	2.48	0.45
1:C:72:GLU:HG3	1:C:73:GLU:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:VAL:HB	1:C:303[A]:LEU:HG	1.98	0.45
1:A:273[B]:ILE:HG22	1:A:283:PRO:HG3	1.96	0.45
1:B:118:VAL:HG22	1:B:165[A]:MET:HE2	1.96	0.45
1:D:44:ASP:OD1	1:D:49:LYS:NZ	2.47	0.45
1:B:118:VAL:HG11	1:B:230[B]:MET:HE2	1.99	0.45
1:B:225:ILE:HG23	1:B:236:PRO:HD2	1.99	0.45
1:B:83:GLU:O	1:B:87[B]:THR:HG23	2.17	0.45
1:A:139:ARG:NH2	1:C:210:LYS:HA	2.33	0.44
1:D:273[A]:ILE:CG2	1:D:283:PRO:HG3	2.48	0.43
1:B:192:PHE:HA	5:B:579:HOH:O	2.18	0.43
1:D:214:TYR:CD2	1:D:280:GLU:HG2	2.53	0.43
1:B:45:GLY:HA3	1:B:47:PHE:CE1	2.53	0.43
1:C:27:ARG:HG2	1:C:29:ASP:HB3	2.01	0.43
1:B:248:LYS:NZ	5:B:507:HOH:O	2.33	0.43
1:A:305:GLU:O	1:A:309:GLU:HG3	2.19	0.42
1:C:65:LYS:NZ	1:C:81:GLU:OE2	2.40	0.42
1:C:118:VAL:HG11	1:C:230[B]:MET:HE2	2.02	0.42
1:B:254:PRO:HA	1:B:255:PRO:HD3	1.93	0.42
1:C:190:ASP:OD1	5:C:504:HOH:O	2.22	0.42
1:C:203:VAL:HG22	1:C:214:TYR:CD1	2.54	0.42
1:C:93[B]:ILE:HD11	1:C:144:ALA:HB1	2.02	0.42
1:A:300:ASN:CG	5:A:502:HOH:O	2.62	0.41
1:C:303[A]:LEU:HD23	1:C:303[A]:LEU:HA	1.89	0.41
1:B:167:LEU:HA	1:B:307:VAL:HG11	2.03	0.41
1:A:291:HIS:CG	1:A:292:PRO:HD2	2.56	0.41
1:D:212:THR:HG22	1:D:214:TYR:H	1.85	0.41
1:B:55:ASN:OD1	1:B:57:GLU:N	2.53	0.40
1:C:188:LYS:HG3	5:C:501:HOH:O	2.21	0.40
1:A:87:THR:HG21	5:D:507:HOH:O	2.20	0.40
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.82	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:649:HOH:O	5:C:673:HOH:O[4_455]	2.01	0.19
5:A:528:HOH:O	5:D:645:HOH:O[4_445]	2.06	0.14

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	282/302 (93%)	274 (97%)	7 (2%)	1 (0%)	30	28
1	B	295/302 (98%)	287 (97%)	8 (3%)	0	100	100
1	C	291/302 (96%)	282 (97%)	9 (3%)	0	100	100
1	D	291/302 (96%)	284 (98%)	7 (2%)	0	100	100
All	All	1159/1208 (96%)	1127 (97%)	31 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU

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	218/259 (84%)	218 (100%)	0	100	100
1	B	233/259 (90%)	231 (99%)	2 (1%)	70	78
1	C	236/259 (91%)	236 (100%)	0	100	100
1	D	240/259 (93%)	236 (98%)	4 (2%)	53	62
All	All	927/1036 (90%)	921 (99%)	6 (1%)	84	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87[A]	THR
1	B	87[B]	THR
1	D	95	LYS
1	D	165[A]	MET
1	D	165[B]	MET
1	D	247	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	33	ASN
1	C	238	HIS
1	D	25	HIS
1	D	238	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	B	208	1	8,10,11	1.77	2 (25%)	10,14,16	1.57	1 (10%)
1	SEP	B	191	1	8,9,10	1.68	2 (25%)	7,12,14	2.03	2 (28%)
1	TPO	B	185	1	8,10,11	1.31	0	10,14,16	1.73	2 (20%)
1	TPO	A	185	1	8,10,11	1.97	3 (37%)	10,14,16	1.15	1 (10%)
1	TPO	C	185	1	8,10,11	1.90	2 (25%)	10,14,16	1.25	1 (10%)
1	TPO	D	185	1	8,10,11	1.67	1 (12%)	10,14,16	1.93	1 (10%)
1	SEP	A	191	1	8,9,10	1.66	1 (12%)	7,12,14	1.39	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	A	208	1	8,10,11	1.55	1 (12%)	10,14,16	1.56	2 (20%)
1	SEP	C	191	1	8,9,10	2.93	5 (62%)	7,12,14	4.63	4 (57%)
1	TPO	C	208	1	8,10,11	1.75	1 (12%)	10,14,16	1.70	1 (10%)
1	SEP	D	191	1	8,9,10	1.65	1 (12%)	7,12,14	1.28	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	B	208	1	-	0/9/11/13	-
1	SEP	B	191	1	-	2/6/8/10	-
1	TPO	B	185	1	-	2/9/11/13	-
1	TPO	A	185	1	-	5/9/11/13	-
1	TPO	C	185	1	-	2/9/11/13	-
1	TPO	D	185	1	-	3/9/11/13	-
1	SEP	A	191	1	-	3/6/8/10	-
1	TPO	A	208	1	-	4/9/11/13	-
1	SEP	C	191	1	-	3/6/8/10	-
1	TPO	C	208	1	-	5/9/11/13	-
1	SEP	D	191	1	-	2/6/8/10	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	191	SEP	P-O3P	4.87	1.72	1.54
1	C	191	SEP	P-O1P	4.82	1.65	1.50
1	C	185	TPO	P-O1P	4.06	1.63	1.50
1	D	185	TPO	P-O1P	3.67	1.61	1.50
1	A	191	SEP	P-O1P	3.62	1.61	1.50
1	C	208	TPO	P-O1P	3.59	1.61	1.50
1	D	191	SEP	P-O1P	3.55	1.61	1.50
1	B	208	TPO	P-O1P	3.54	1.61	1.50
1	B	191	SEP	P-O1P	3.54	1.61	1.50
1	A	185	TPO	P-O1P	3.47	1.61	1.50
1	A	208	TPO	P-O1P	3.11	1.60	1.50
1	C	191	SEP	P-O2P	3.08	1.66	1.54
1	A	185	TPO	P-OG1	2.29	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	TPO	CB-CA	2.27	1.58	1.53
1	C	191	SEP	OG-CB	2.26	1.53	1.44
1	B	208	TPO	P-O3P	2.18	1.62	1.54
1	C	191	SEP	CB-CA	2.06	1.57	1.52
1	B	191	SEP	P-O3P	2.02	1.62	1.54
1	C	185	TPO	P-OG1	2.00	1.63	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	SEP	OG-CB-CA	9.73	117.61	108.14
1	C	191	SEP	O3P-P-OG	5.64	121.37	106.67
1	D	185	TPO	P-OG1-CB	-5.61	108.07	123.33
1	C	208	TPO	P-OG1-CB	-4.83	110.19	123.33
1	B	208	TPO	P-OG1-CB	-4.39	111.39	123.33
1	B	191	SEP	OG-CB-CA	4.15	112.18	108.14
1	B	185	TPO	P-OG1-CB	-4.09	112.21	123.33
1	A	208	TPO	CG2-CB-CA	-3.88	105.71	113.26
1	C	191	SEP	OG-P-O1P	3.68	116.39	106.44
1	A	191	SEP	OG-CB-CA	2.85	110.92	108.14
1	C	191	SEP	O3P-P-O1P	-2.62	100.62	110.83
1	B	185	TPO	CG2-CB-CA	-2.61	108.17	113.26
1	B	191	SEP	OG-P-O1P	2.53	113.27	106.44
1	A	208	TPO	O3P-P-OG1	2.52	115.68	105.85
1	D	191	SEP	OG-CB-CA	2.39	110.47	108.14
1	C	185	TPO	P-OG1-CB	-2.24	117.23	123.33
1	A	185	TPO	P-OG1-CB	-2.04	117.78	123.33

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	185	TPO	N-CA-CB-OG1
1	B	191	SEP	N-CA-CB-OG
1	B	191	SEP	C-CA-CB-OG
1	A	185	TPO	N-CA-CB-CG2
1	A	185	TPO	N-CA-CB-OG1
1	A	185	TPO	C-CA-CB-CG2
1	A	185	TPO	O-C-CA-CB
1	A	185	TPO	CA-CB-OG1-P
1	A	191	SEP	N-CA-CB-OG
1	A	191	SEP	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	A	208	TPO	N-CA-CB-CG2
1	A	208	TPO	N-CA-CB-OG1
1	A	208	TPO	C-CA-CB-CG2
1	A	208	TPO	CG2-CB-OG1-P
1	C	185	TPO	CA-CB-OG1-P
1	C	191	SEP	N-CA-CB-OG
1	C	191	SEP	C-CA-CB-OG
1	C	208	TPO	N-CA-CB-OG1
1	D	185	TPO	N-CA-CB-CG2
1	D	185	TPO	N-CA-CB-OG1
1	D	185	TPO	C-CA-CB-CG2
1	D	191	SEP	CA-CB-OG-P
1	C	208	TPO	C-CA-CB-CG2
1	A	191	SEP	CB-OG-P-O1P
1	D	191	SEP	N-CA-CB-OG
1	C	208	TPO	N-CA-CB-CG2
1	C	208	TPO	CA-CB-OG1-P
1	C	191	SEP	CB-OG-P-O3P
1	B	185	TPO	O-C-CA-CB
1	C	185	TPO	O-C-CA-CB
1	C	208	TPO	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	208	TPO	1	0
1	A	185	TPO	1	0
1	C	185	TPO	1	0
1	C	191	SEP	1	0
1	C	208	TPO	1	0
1	D	191	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	EDO	D	403	-	3,3,3	0.55	0	2,2,2	0.47	0
3	EDO	D	404	-	3,3,3	0.62	0	2,2,2	0.19	0
2	R70	C	401	-	32,33,33	0.36	0	40,46,46	0.57	1 (2%)
3	EDO	B	403	-	3,3,3	0.37	0	2,2,2	0.80	0
3	EDO	C	402	-	3,3,3	0.58	0	2,2,2	0.08	0
2	R70	A	401	-	32,33,33	0.24	0	40,46,46	0.45	0
2	R70	D	401	-	32,33,33	0.36	0	40,46,46	0.60	0
3	EDO	B	404	-	3,3,3	0.60	0	2,2,2	0.07	0
3	EDO	D	402	-	3,3,3	0.31	0	2,2,2	0.62	0
2	R70	B	401	-	32,33,33	0.27	0	40,46,46	0.41	0
3	EDO	B	402	-	3,3,3	0.67	0	2,2,2	0.36	0
3	EDO	B	405	-	3,3,3	0.45	0	2,2,2	0.54	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	EDO	D	403	-	-	1/1/1/1	-
3	EDO	D	404	-	-	0/1/1/1	-
2	R70	C	401	-	-	0/18/34/34	0/4/4/4
3	EDO	B	403	-	-	0/1/1/1	-
3	EDO	C	402	-	-	0/1/1/1	-
2	R70	A	401	-	-	0/18/34/34	0/4/4/4
2	R70	D	401	-	-	0/18/34/34	0/4/4/4
3	EDO	B	404	-	-	0/1/1/1	-
3	EDO	D	402	-	-	0/1/1/1	-
2	R70	B	401	-	-	0/18/34/34	0/4/4/4
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	B	405	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	R70	C9-C8-N1	-2.55	116.15	122.29

There are no chirality outliers.

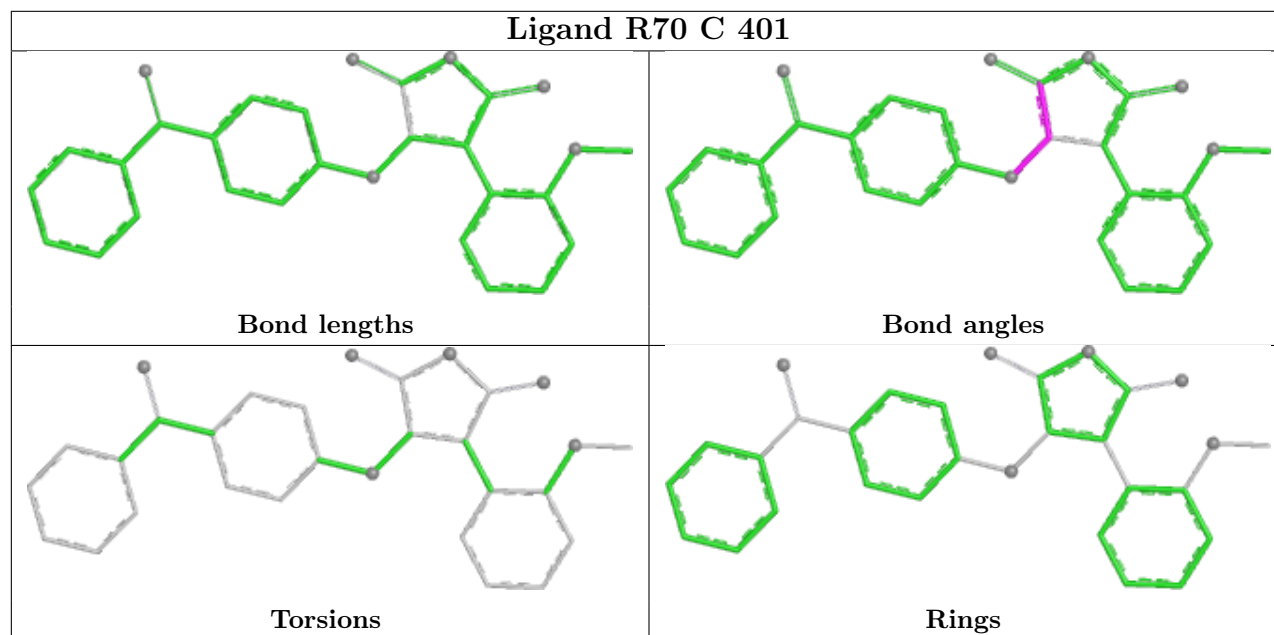
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	403	EDO	O1-C1-C2-O2

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	282/302 (93%)	0.67	47 (16%) 4 4	17, 47, 110, 126	5 (1%)
1	B	288/302 (95%)	0.36	42 (14%) 6 6	15, 37, 105, 131	9 (3%)
1	C	285/302 (94%)	0.60	42 (14%) 6 6	14, 43, 94, 118	10 (3%)
1	D	285/302 (94%)	0.20	25 (8%) 15 16	16, 37, 84, 111	10 (3%)
All	All	1140/1208 (94%)	0.45	156 (13%) 6 7	14, 41, 103, 131	34 (2%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	183	LEU	6.9
1	A	187	GLN	6.9
1	B	47	PHE	6.0
1	A	184	LYS	5.9
1	C	193	ILE	5.8
1	C	194	GLY	5.7
1	A	69	THR	5.7
1	C	181	LYS	5.5
1	C	47	PHE	5.2
1	D	193[A]	ILE	5.2
1	C	186	LEU	5.1
1	C	212	THR	5.1
1	A	102	HIS	5.1
1	A	104	GLY	5.1
1	B	314	VAL	5.1
1	C	211	ASP	5.1
1	C	46	ALA	4.9
1	A	47	PHE	4.9
1	D	190	ASP	4.9
1	B	69	THR	4.8
1	A	30	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	73	GLU	4.7
1	C	189	ARG	4.7
1	D	212	THR	4.6
1	C	214	TYR	4.6
1	B	102	HIS	4.5
1	C	192	PHE	4.4
1	A	103	ASP	4.4
1	A	24	GLU	4.3
1	D	186	LEU	4.3
1	A	313	GLU	4.3
1	C	180	ALA	4.1
1	D	312	ALA	4.1
1	B	30	LEU	4.1
1	C	75	LEU	4.1
1	D	23	TYR	4.1
1	C	70	LYS	4.1
1	C	312	ALA	4.0
1	A	186	LEU	4.0
1	C	77	ASP	4.0
1	C	188	LYS	4.0
1	D	207	GLU	4.0
1	B	34	GLU	3.9
1	A	101	TYR	3.9
1	C	184	LYS	3.9
1	A	72	GLU	3.8
1	A	77	ASP	3.8
1	D	211	ASP	3.8
1	A	58	THR	3.8
1	D	183	LEU	3.8
1	A	183	LEU	3.7
1	A	312	ALA	3.6
1	C	80	VAL	3.6
1	C	187	GLN	3.6
1	B	73	GLU	3.5
1	D	206	CYS	3.5
1	B	58	THR	3.5
1	A	66	VAL	3.5
1	A	25	HIS	3.4
1	C	182	ASN	3.4
1	A	192	PHE	3.3
1	B	48	GLY	3.3
1	A	74	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	46	ALA	3.2
1	B	57	GLU	3.2
1	A	75	LEU	3.2
1	B	68	GLU	3.2
1	D	77	ASP	3.1
1	B	190	ASP	3.1
1	C	213	PRO	3.1
1	B	74	GLU	3.1
1	C	25	HIS	3.1
1	A	67	ILE	3.1
1	A	105	LYS	3.1
1	C	210	LYS	3.1
1	A	38	ILE	3.1
1	C	78	TYR	3.0
1	D	76	GLU	3.0
1	D	188	LYS	3.0
1	B	46	ALA	3.0
1	D	189	ARG	3.0
1	A	78	TYR	3.0
1	B	67	ILE	3.0
1	C	26	VAL	3.0
1	D	311	LYS	2.9
1	C	30	LEU	2.9
1	C	69	THR	2.8
1	C	79	ILE	2.8
1	D	47	PHE	2.8
1	B	186	LEU	2.8
1	A	29	ASP	2.8
1	A	68	GLU	2.7
1	C	241	ASN	2.7
1	B	78	TYR	2.7
1	B	75	LEU	2.7
1	B	76	GLU	2.7
1	A	57	GLU	2.7
1	C	44	ASP	2.7
1	B	188	LYS	2.7
1	D	78	TYR	2.6
1	B	24	GLU	2.6
1	B	72	GLU	2.6
1	A	182	ASN	2.6
1	C	48	GLY	2.6
1	B	26	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	59	GLY	2.5
1	D	46	ALA	2.5
1	A	37	GLU	2.5
1	A	76	GLU	2.5
1	B	101	TYR	2.5
1	A	100	TYR	2.5
1	B	71	SER	2.5
1	D	187	GLN	2.5
1	C	28	ARG	2.5
1	D	213	PRO	2.5
1	B	106	LEU	2.5
1	A	27	ARG	2.5
1	B	45	GLY	2.5
1	B	187	GLN	2.4
1	A	73	GLU	2.4
1	A	107	TRP	2.4
1	B	39	VAL	2.4
1	A	61	LEU	2.4
1	C	209	MET	2.4
1	C	45	GLY	2.3
1	B	70	LYS	2.3
1	D	27	ARG	2.3
1	A	298	THR	2.3
1	D	73	GLU	2.3
1	C	76	GLU	2.3
1	A	28	ARG	2.3
1	D	184	LYS	2.3
1	A	26	VAL	2.3
1	B	107	TRP	2.3
1	C	58	THR	2.2
1	D	24	GLU	2.2
1	B	32	PRO	2.2
1	A	56	LYS	2.2
1	B	41	GLU	2.2
1	C	195	THR	2.2
1	B	103	ASP	2.2
1	A	34	GLU	2.2
1	A	89	ASP	2.1
1	C	215	ASP	2.1
1	B	192	PHE	2.1
1	A	59	GLY	2.1
1	C	243[A]	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	25	HIS	2.1
1	A	43	GLY	2.1
1	B	105	LYS	2.0
1	B	104	GLY	2.0
1	A	35	VAL	2.0
1	B	36	TRP	2.0
1	B	29	ASP	2.0
1	B	27	ARG	2.0
1	D	25	HIS	2.0

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

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
1	SEP	A	191	10/11	0.51	0.15	80,102,124,124	0
1	TPO	D	185	11/12	0.51	0.22	106,120,127,127	0
1	SEP	C	191	10/11	0.56	0.30	72,96,113,114	0
1	TPO	C	185	11/12	0.56	0.22	112,125,134,138	0
1	TPO	A	185	11/12	0.62	0.21	89,98,107,116	0
1	SEP	D	191	10/11	0.72	0.15	83,97,113,114	0
1	TPO	C	208	11/12	0.75	0.17	75,84,112,115	0
1	SEP	B	191	10/11	0.76	0.14	74,84,89,91	0
1	TPO	A	208	11/12	0.93	0.10	41,56,76,76	0
1	TPO	B	185	11/12	0.94	0.08	52,56,68,75	0
1	TPO	B	208	11/12	0.95	0.08	40,47,62,81	0

6.3 Carbohydrates ⓘ

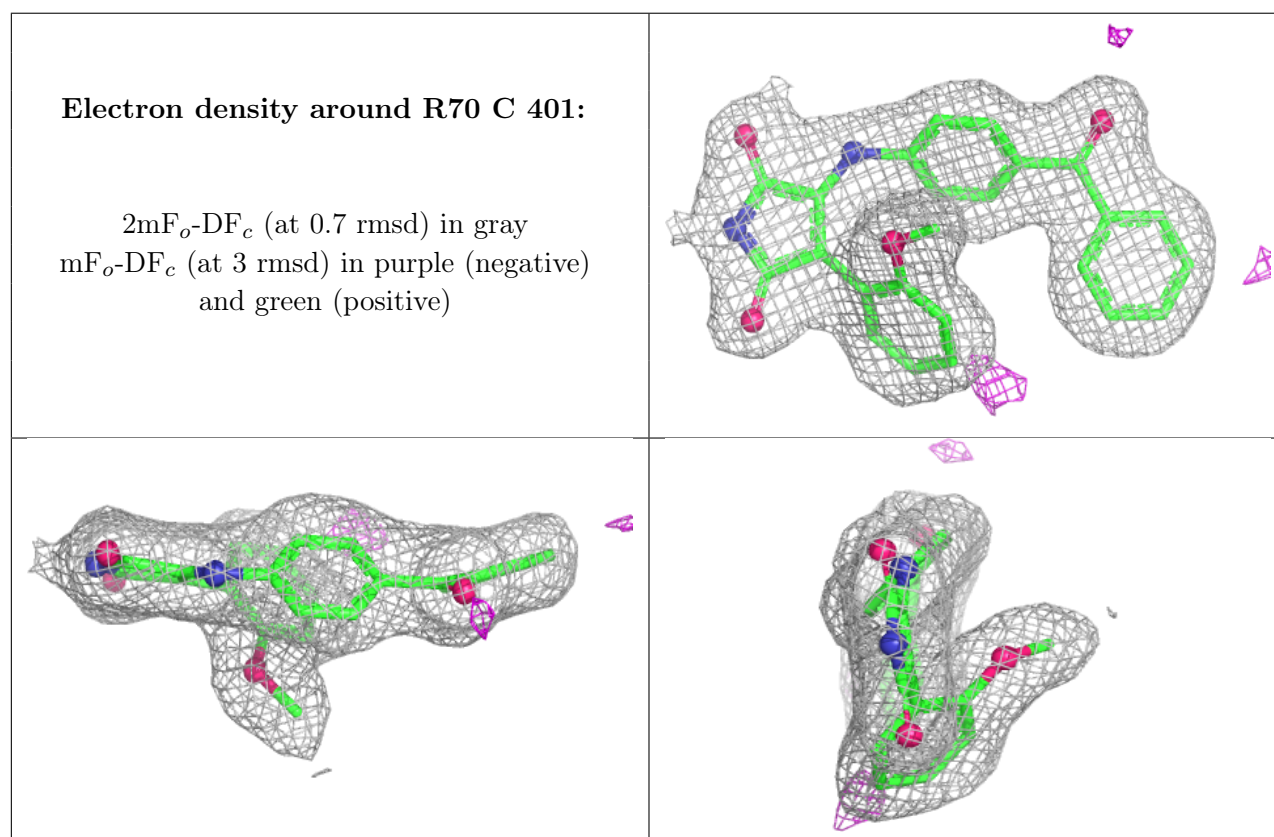
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	EDO	B	404	4/4	0.85	0.28	64,70,73,74	0
3	EDO	D	403	4/4	0.89	0.16	51,53,54,55	0
3	EDO	B	402	4/4	0.93	0.12	39,45,45,47	0
3	EDO	B	403	4/4	0.93	0.11	34,35,42,48	0
3	EDO	C	402	4/4	0.94	0.13	53,57,57,59	0
2	R70	A	401	30/30	0.94	0.10	41,49,62,63	0
2	R70	B	401	30/30	0.95	0.08	34,39,48,51	0
3	EDO	B	405	4/4	0.95	0.12	44,49,55,64	0
4	CL	A	402	1/1	0.95	0.12	68,68,68,68	0
3	EDO	D	404	4/4	0.96	0.10	41,42,47,48	0
2	R70	D	401	30/30	0.97	0.06	25,33,38,42	0
2	R70	C	401	30/30	0.97	0.07	32,36,40,42	0
3	EDO	D	402	4/4	0.97	0.09	31,37,46,54	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.