



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:05 PM UTC

PDB ID : 8UL8 / pdb_00008ul8
Title : LSD1-CoREST in complex with T15, short soaking
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2023-10-16
Resolution : 2.82 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

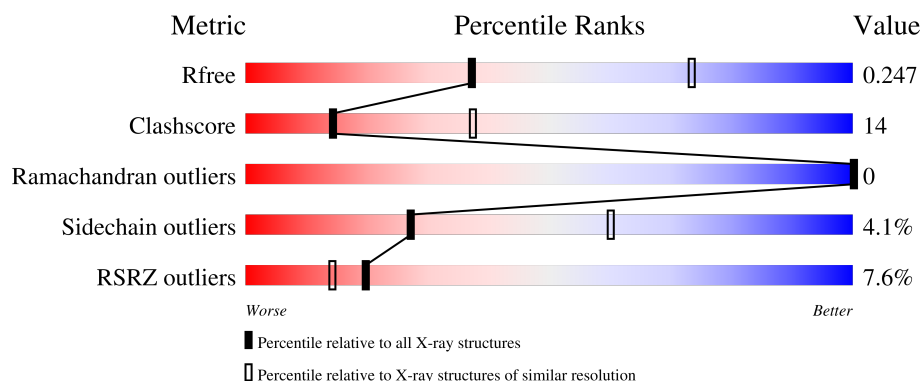
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	871	4% 55% 20% • 24%
2	B	144	19% 55% 33% • • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6360 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 Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5217	3324	906	967	20			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O60341
A	-17	SER	-	expression tag	UNP O60341
A	-16	SER	-	expression tag	UNP O60341
A	-15	HIS	-	expression tag	UNP O60341
A	-14	HIS	-	expression tag	UNP O60341
A	-13	HIS	-	expression tag	UNP O60341
A	-12	HIS	-	expression tag	UNP O60341
A	-11	HIS	-	expression tag	UNP O60341
A	-10	HIS	-	expression tag	UNP O60341
A	-9	SER	-	expression tag	UNP O60341
A	-8	SER	-	expression tag	UNP O60341
A	-7	GLY	-	expression tag	UNP O60341
A	-6	LEU	-	expression tag	UNP O60341
A	-5	VAL	-	expression tag	UNP O60341
A	-4	PRO	-	expression tag	UNP O60341
A	-3	ARG	-	expression tag	UNP O60341
A	-2	GLY	-	expression tag	UNP O60341
A	-1	SER	-	expression tag	UNP O60341
A	0	HIS	-	expression tag	UNP O60341

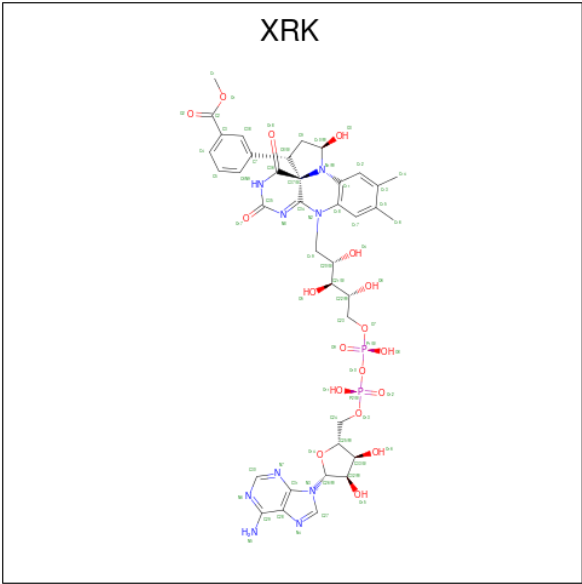
- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	GLY	-	expression tag	UNP Q9UKL0
B	298	PRO	-	expression tag	UNP Q9UKL0
B	299	LEU	-	expression tag	UNP Q9UKL0
B	300	GLY	-	expression tag	UNP Q9UKL0
B	301	SER	-	expression tag	UNP Q9UKL0
B	302	PRO	-	expression tag	UNP Q9UKL0
B	303	GLU	-	expression tag	UNP Q9UKL0
B	304	PHE	-	expression tag	UNP Q9UKL0

- Molecule 3 is methyl 3-{(1R,3S,3aS,13R)-8-[(2S,3S,4R)-5-{{(S)-{[(S)-{[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]oxy}-2,3,4-trihydroxypentyl]-1-hydroxy-10,11-dimethyl-4,6-dioxo-2,3,4,5,6,8-hexahydro-1H-benzo[g]pyrrolo[2,1-e]pteridin-3-yl}benzoate (non-preferred name) (CCD ID: XRK) (formula: C₃₈H₄₅N₉O₁₈P₂) (labeled as "Ligand of Interest" by depositor).

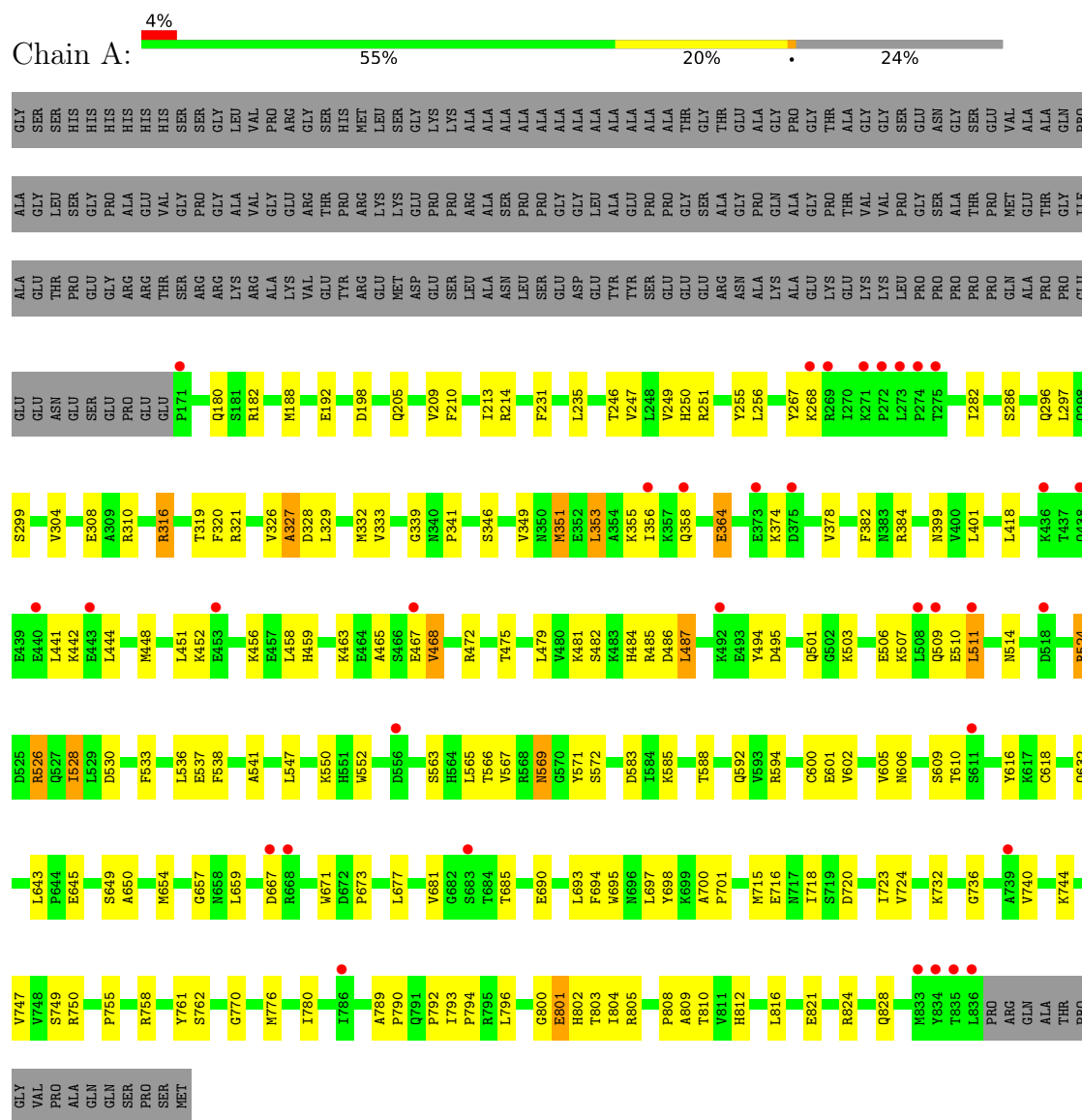


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			67	38	9	18	2		

3 Residue-property plots

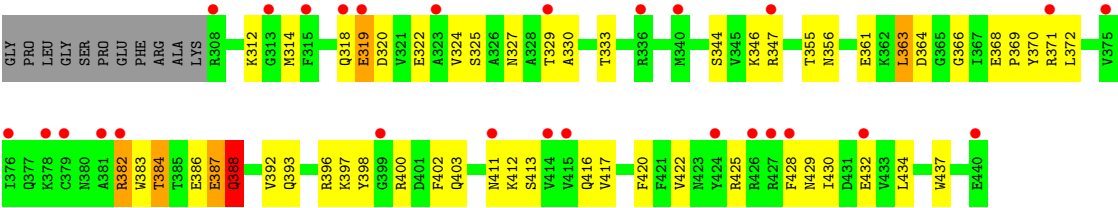
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Lysine-specific histone demethylase 1A



• Molecule 2: REST corepressor 1





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.53Å 178.97Å 235.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 2.82 48.54 – 2.82	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.54-2.82) 96.5 (48.54-2.82)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.224 , 0.247 0.227 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å ²)	82.1	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.1	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	6360	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: X RK

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	0.67	1/5331 (0.0%)	0.90	13/7232 (0.2%)
2	B	0.65	0/1091	1.03	5/1471 (0.3%)
All	All	0.66	1/6422 (0.0%)	0.92	18/8703 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	LYS	CG-CD	6.41	1.71	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	LYS	CA-CB-CG	10.18	134.46	114.10
1	A	468	VAL	CA-C-N	-6.52	101.70	121.98
1	A	468	VAL	C-N-CA	-6.52	101.70	121.98
1	A	268	LYS	N-CA-CB	6.31	119.58	110.06
2	B	319	GLU	CA-C-N	-6.15	110.21	121.52
2	B	319	GLU	C-N-CA	-6.15	110.21	121.52
1	A	327	ALA	CA-C-N	-5.61	113.40	121.42
1	A	327	ALA	C-N-CA	-5.61	113.40	121.42
1	A	316	ARG	CB-CG-CD	5.50	123.94	111.30
2	B	346	LYS	CA-C-N	-5.21	112.91	121.92
2	B	346	LYS	C-N-CA	-5.21	112.91	121.92
1	A	792	PRO	CA-C-N	5.20	131.75	122.13
1	A	792	PRO	C-N-CA	5.20	131.75	122.13
1	A	267	TYR	CA-C-N	-5.20	113.99	121.42
1	A	267	TYR	C-N-CA	-5.20	113.99	121.42
2	B	388	GLN	CB-CA-C	-5.15	102.79	110.88
1	A	800	GLY	CA-C-O	-5.09	118.66	122.37
1	A	803	THR	CA-CB-OG1	-5.03	102.05	109.60

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	5217	0	5252	143	0
2	B	1076	0	1091	52	0
3	A	67	0	0	1	0
All	All	6360	0	6343	179	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 14.

All (179) 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:346:SER:HA	1:A:351:MET:CE	1.65	1.25
1:A:346:SER:HA	1:A:351:MET:HE2	1.28	1.16
2:B:388:GLN:HG2	2:B:428:PHE:HE2	1.20	1.06
2:B:388:GLN:HG2	2:B:428:PHE:CE2	1.90	1.04
2:B:382:ARG:HH21	2:B:382:ARG:HB2	1.25	0.99
1:A:346:SER:CA	1:A:351:MET:CE	2.41	0.98
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.53	0.89
2:B:382:ARG:HH21	2:B:382:ARG:CB	1.91	0.84
2:B:368:GLU:OE2	2:B:371:ARG:NH1	2.13	0.82
2:B:396:ARG:HH11	2:B:396:ARG:HG3	1.43	0.82
1:A:716:GLU:HG2	1:A:750:ARG:HG2	1.60	0.81
1:A:384:ARG:NH2	2:B:312:LYS:O	2.12	0.81
1:A:384:ARG:HB3	2:B:314:MET:HE3	1.62	0.81
1:A:448:MET:HE2	2:B:363:LEU:CD1	2.11	0.81
1:A:583:ASP:OD2	1:A:585:LYS:NZ	2.14	0.79
1:A:316:ARG:NH1	3:A:901:XRK:O12	2.17	0.77
1:A:511:LEU:HD23	1:A:511:LEU:N	2.01	0.74
1:A:448:MET:HE2	2:B:363:LEU:HD12	1.70	0.73
1:A:526:ARG:CG	1:A:526:ARG:HH11	2.02	0.73
1:A:569:ASN:OD1	1:A:569:ASN:N	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:SER:CB	1:A:351:MET:CE	2.66	0.73
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.54	0.72
2:B:396:ARG:HG3	2:B:396:ARG:NH1	2.05	0.70
1:A:346:SER:CA	1:A:351:MET:HE1	2.20	0.70
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.75	0.68
2:B:319:GLU:HG3	2:B:320:ASP:OD1	1.93	0.68
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.29	0.67
1:A:308:GLU:OE1	1:A:310:ARG:N	2.29	0.65
1:A:801:GLU:HG3	1:A:809:ALA:CA	2.27	0.65
1:A:346:SER:HB2	1:A:351:MET:HE3	1.79	0.65
2:B:382:ARG:HB2	2:B:382:ARG:NH2	2.07	0.64
2:B:361:GLU:OE1	2:B:361:GLU:HA	1.98	0.64
1:A:382:PHE:HZ	1:A:536:LEU:HD13	1.64	0.63
1:A:606:ASN:HD22	1:A:609:SER:H	1.46	0.63
1:A:463:LYS:O	1:A:467:GLU:HG2	1.99	0.62
1:A:316:ARG:NH2	1:A:801:GLU:OE2	2.32	0.62
1:A:353:LEU:HD13	1:A:565:LEU:HD22	1.80	0.62
2:B:384:THR:H	2:B:387:GLU:HG3	1.64	0.62
1:A:821:GLU:OE1	1:A:824:ARG:HD3	2.00	0.62
1:A:356:ILE:HD11	1:A:358:GLN:OE1	2.01	0.61
1:A:346:SER:CB	1:A:351:MET:HE3	2.30	0.61
1:A:442:LYS:HE2	2:B:355:THR:HG21	1.82	0.61
1:A:346:SER:CB	1:A:351:MET:HE1	2.31	0.60
1:A:632:GLN:NE2	1:A:758:ARG:HH21	1.99	0.60
1:A:452:LYS:HE3	2:B:366:GLY:O	2.01	0.60
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.65	0.59
1:A:732:LYS:O	1:A:736:GLY:N	2.30	0.59
1:A:468:VAL:O	1:A:472:ARG:NH2	2.36	0.59
1:A:645:GLU:OE2	1:A:649:SER:OG	2.20	0.58
1:A:793:ILE:HD12	1:A:793:ILE:H	1.68	0.58
2:B:382:ARG:HH21	2:B:382:ARG:CG	2.17	0.58
2:B:403:GLN:OE1	2:B:403:GLN:HA	2.04	0.57
1:A:444:LEU:HD21	1:A:501:GLN:HB2	1.86	0.57
1:A:319:THR:HB	1:A:572:SER:HB3	1.86	0.57
1:A:804:ILE:O	1:A:804:ILE:HG23	2.03	0.57
1:A:441:LEU:HG	2:B:356:ASN:ND2	2.19	0.56
2:B:388:GLN:CG	2:B:428:PHE:HE2	2.07	0.56
2:B:383:TRP:CZ2	2:B:420:PHE:HB2	2.41	0.56
2:B:383:TRP:CH2	2:B:420:PHE:CD1	2.94	0.55
1:A:378:VAL:HG11	1:A:528:ILE:HG22	1.87	0.55
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:PHE:O	1:A:537:GLU:HG3	2.06	0.54
1:A:346:SER:HA	1:A:351:MET:HE3	1.80	0.54
1:A:821:GLU:OE1	1:A:821:GLU:HA	2.06	0.54
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.90	0.54
1:A:507:LYS:O	1:A:511:LEU:HG	2.07	0.54
1:A:286:SER:H	1:A:308:GLU:HG2	1.73	0.54
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.43	0.53
1:A:205:GLN:O	1:A:209:VAL:HG23	2.09	0.53
1:A:667:ASP:HB3	1:A:744:LYS:HE3	1.92	0.52
2:B:382:ARG:NH2	2:B:382:ARG:CG	2.73	0.52
1:A:188:MET:HE3	1:A:210:PHE:CE2	2.45	0.52
2:B:413:SER:O	2:B:417:VAL:HG23	2.10	0.52
1:A:762:SER:OG	1:A:801:GLU:OE1	2.22	0.51
1:A:209:VAL:O	1:A:213:ILE:HG13	2.10	0.51
2:B:398:TYR:O	2:B:437:TRP:CE2	2.63	0.51
1:A:609:SER:O	1:A:609:SER:OG	2.23	0.51
1:A:329:LEU:HD12	1:A:749:SER:HB3	1.91	0.51
1:A:695:TRP:HB3	1:A:697:LEU:HG	1.92	0.51
1:A:465:ALA:HB2	1:A:479:LEU:HD23	1.92	0.51
1:A:755:PRO:HA	1:A:758:ARG:NH1	2.25	0.51
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.26	0.50
1:A:503:LYS:O	1:A:506:GLU:HG2	2.12	0.50
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.76	0.50
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.93	0.50
1:A:600:CYS:HB2	1:A:618:CYS:SG	2.51	0.50
2:B:400:ARG:HA	2:B:402:PHE:CE2	2.47	0.49
1:A:762:SER:CB	1:A:801:GLU:OE1	2.61	0.49
1:A:192:GLU:OE1	1:A:214:ARG:NE	2.46	0.49
1:A:328:ASP:OD2	1:A:571:TYR:HB2	2.13	0.49
2:B:413:SER:N	2:B:416:GLN:OE1	2.40	0.48
1:A:567:VAL:HG11	1:A:571:TYR:HA	1.96	0.48
1:A:401:LEU:HD11	2:B:325:SER:HB2	1.96	0.48
1:A:650:ALA:O	1:A:654:MET:HG3	2.14	0.48
2:B:384:THR:N	2:B:387:GLU:HG3	2.28	0.48
1:A:235:LEU:HD21	1:A:246:THR:HG22	1.96	0.47
1:A:198:ASP:N	1:A:198:ASP:OD1	2.46	0.47
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.96	0.47
2:B:363:LEU:HD23	2:B:363:LEU:N	2.28	0.47
1:A:541:ALA:O	1:A:657:GLY:HA3	2.13	0.47
1:A:794:PRO:HD2	1:A:828:GLN:NE2	2.29	0.47
1:A:802:HIS:ND1	1:A:802:HIS:N	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.95	0.47
1:A:671:TRP:O	1:A:673:PRO:HD3	2.14	0.47
1:A:319:THR:CB	1:A:572:SER:HB3	2.44	0.47
1:A:485:ARG:C	1:A:485:ARG:HD3	2.40	0.46
1:A:355:LYS:NZ	1:A:563:SER:HB2	2.30	0.46
2:B:388:GLN:HG2	2:B:428:PHE:CZ	2.46	0.46
2:B:425:ARG:HA	2:B:430:ILE:HD12	1.98	0.46
1:A:693:LEU:HD23	1:A:694:PHE:H	1.81	0.46
1:A:690:GLU:OE2	1:A:715:MET:HE3	2.15	0.46
1:A:346:SER:O	1:A:349:VAL:O	2.34	0.45
1:A:776:MET:HE2	1:A:802:HIS:HD2	1.80	0.45
1:A:296:GLN:O	1:A:299:SER:HB3	2.17	0.45
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.97	0.45
1:A:793:ILE:HG23	1:A:828:GLN:OE1	2.17	0.45
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.99	0.45
1:A:321:ARG:HG2	1:A:326:VAL:HG22	1.98	0.45
1:A:808:PRO:O	1:A:810:THR:HG23	2.16	0.45
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.82	0.44
1:A:286:SER:OG	1:A:308:GLU:HG3	2.18	0.44
1:A:677:LEU:HB2	1:A:693:LEU:HD21	2.00	0.44
1:A:789:ALA:HB1	1:A:790:PRO:HD2	1.99	0.44
2:B:434:LEU:HD23	2:B:434:LEU:HA	1.68	0.44
2:B:429:ASN:ND2	2:B:432:GLU:OE1	2.51	0.44
1:A:255:TYR:CE2	1:A:256:LEU:HD23	2.53	0.44
1:A:341:PRO:HG3	1:A:816:LEU:HD21	1.99	0.44
1:A:418:LEU:HD21	2:B:324:VAL:HG21	2.00	0.44
1:A:720:ASP:O	1:A:724:VAL:HG23	2.18	0.44
1:A:801:GLU:CG	1:A:809:ALA:H	2.31	0.44
1:A:677:LEU:HA	1:A:694:PHE:O	2.18	0.43
1:A:182:ARG:NH1	1:A:341:PRO:HD3	2.34	0.43
2:B:329:THR:O	2:B:333:THR:HG23	2.17	0.43
1:A:601:GLU:HA	1:A:616:TYR:O	2.18	0.43
1:A:297:LEU:HB2	1:A:304:VAL:HG21	2.00	0.43
1:A:762:SER:N	1:A:801:GLU:OE1	2.52	0.43
1:A:538:PHE:HD1	1:A:659:LEU:HD22	1.83	0.43
2:B:422:VAL:HA	2:B:425:ARG:HB2	2.00	0.43
1:A:364:GLU:HA	1:A:681:VAL:HB	2.00	0.43
1:A:812:HIS:O	1:A:816:LEU:HG	2.19	0.43
1:A:231:PHE:CZ	1:A:250:HIS:HB2	2.54	0.43
2:B:370:TYR:CD2	2:B:370:TYR:N	2.87	0.43
1:A:524:ARG:O	1:A:528:ILE:HD12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:ILE:HB	1:A:796:LEU:HB3	2.00	0.42
2:B:411:ASN:C	2:B:412:LYS:HG2	2.44	0.42
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.89	0.42
1:A:441:LEU:HG	2:B:356:ASN:HD22	1.84	0.42
1:A:770:GLY:O	1:A:805:ARG:HG3	2.19	0.42
1:A:526:ARG:HH11	1:A:526:ARG:HG2	1.82	0.42
1:A:700:ALA:HB1	1:A:701:PRO:HD2	2.01	0.42
1:A:198:ASP:OD2	1:A:251:ARG:NH2	2.52	0.42
1:A:399:ASN:ND2	1:A:550:LYS:HE2	2.35	0.42
1:A:401:LEU:HD12	1:A:401:LEU:HA	1.82	0.42
1:A:459:HIS:HB2	1:A:487:LEU:HD11	2.01	0.42
1:A:530:ASP:OD2	1:A:685:THR:HA	2.20	0.42
1:A:475:THR:HA	2:B:393:GLN:HE22	1.85	0.42
1:A:594:ARG:HB2	1:A:601:GLU:HG3	2.02	0.42
1:A:486:ASP:OD1	2:B:397:LYS:NZ	2.53	0.41
1:A:632:GLN:NE2	1:A:758:ARG:NH2	2.68	0.41
2:B:318:GLN:O	2:B:322:GLU:HG3	2.21	0.41
1:A:356:ILE:HD11	1:A:358:GLN:CD	2.45	0.41
1:A:485:ARG:HD3	1:A:486:ASP:N	2.35	0.41
1:A:495:ASP:OD2	2:B:371:ARG:NH2	2.54	0.41
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.56	0.41
1:A:320:PHE:CD1	1:A:747:VAL:HG21	2.56	0.41
2:B:383:TRP:CZ3	2:B:420:PHE:CD1	3.09	0.41
1:A:247:VAL:O	1:A:251:ARG:HB2	2.20	0.41
1:A:654:MET:HE2	1:A:654:MET:HB3	1.70	0.41
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.82	0.40
1:A:643:LEU:HD23	1:A:643:LEU:HA	1.77	0.40
1:A:458:LEU:HD21	1:A:486:ASP:HB3	2.02	0.40
1:A:251:ARG:HH11	1:A:251:ARG:HD2	1.75	0.40
1:A:332:MET:HG3	1:A:333:VAL:HG23	2.03	0.40
2:B:344:SER:O	2:B:347:ARG:HD3	2.21	0.40
2:B:368:GLU:N	2:B:369:PRO:CD	2.85	0.40
1:A:327:ALA:HA	1:A:698:TYR:CZ	2.57	0.40
1:A:465:ALA:CB	1:A:479:LEU:HD23	2.51	0.40
1:A:801:GLU:HG2	1:A:809:ALA:H	1.87	0.40
1:A:740:VAL:HG13	1:A:740:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	664/871 (76%)	638 (96%)	26 (4%)	0	100	100
2	B	131/144 (91%)	119 (91%)	12 (9%)	0	100	100
All	All	795/1015 (78%)	757 (95%)	38 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/715 (79%)	546 (96%)	20 (4%)	32	65
2	B	117/125 (94%)	109 (93%)	8 (7%)	14	40
All	All	683/840 (81%)	655 (96%)	28 (4%)	27	60

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	MET
1	A	353	LEU
1	A	364	GLU
1	A	374	LYS
1	A	481	LYS
1	A	482	SER
1	A	487	LEU
1	A	509	GLN

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Mol	Chain	Res	Type
1	A	510	GLU
1	A	511	LEU
1	A	514	ASN
1	A	524	ARG
1	A	526	ARG
1	A	528	ILE
1	A	569	ASN
1	A	588	THR
1	A	592	GLN
1	A	605	VAL
1	A	610	THR
1	A	801	GLU
2	B	363	LEU
2	B	364	ASP
2	B	382	ARG
2	B	384	THR
2	B	386	GLU
2	B	387	GLU
2	B	388	GLN
2	B	392	VAL

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

Mol	Chain	Res	Type
1	A	259	HIS
1	A	298	GLN
1	A	399	ASN
1	A	417	GLN
1	A	460	GLN
1	A	484	HIS
1	A	514	ASN
1	A	532	HIS
1	A	632	GLN
1	A	742	GLN
1	A	806	ASN
1	A	828	GLN
2	B	327	ASN
2	B	393	GLN
2	B	429	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	XRK	A	901	-	71,74,74	1.31	10 (14%)	97,115,115	1.35	6 (6%)

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	XRK	A	901	-	-	8/44/112/112	0/7/8/8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	XRK	C35-N8	-3.21	1.29	1.36
3	A	901	XRK	C36-N9	-3.20	1.32	1.37
3	A	901	XRK	O4-C20	-3.13	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	XRK	C11-N1	-2.77	1.36	1.41
3	A	901	XRK	P2-O10	-2.37	1.56	1.59
3	A	901	XRK	O5-C21	-2.30	1.37	1.43
3	A	901	XRK	O17-C35	-2.29	1.19	1.24
3	A	901	XRK	P2-O11	-2.09	1.45	1.55
3	A	901	XRK	P1-O8	-2.05	1.45	1.55
3	A	901	XRK	C19-C20	-2.02	1.49	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	XRK	C37-C8-C7	7.99	128.48	116.08
3	A	901	XRK	C11-N1-C10	-4.82	112.86	123.92
3	A	901	XRK	C36-C37-C34	-3.99	106.33	113.40
3	A	901	XRK	C36-N9-C35	-3.34	120.38	125.42
3	A	901	XRK	C8-C9-C10	-2.57	99.07	104.25
3	A	901	XRK	C9-C8-C7	2.15	120.78	116.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	XRK	O6-C22-C23-O7
3	A	901	XRK	P2-O10-P1-O7
3	A	901	XRK	C3-C2-O1-C1
3	A	901	XRK	O2-C2-O1-C1
3	A	901	XRK	O4-C20-C21-C22
3	A	901	XRK	C21-C22-C23-O7
3	A	901	XRK	C32-C26-N3-C27
3	A	901	XRK	O2-C2-C3-C4

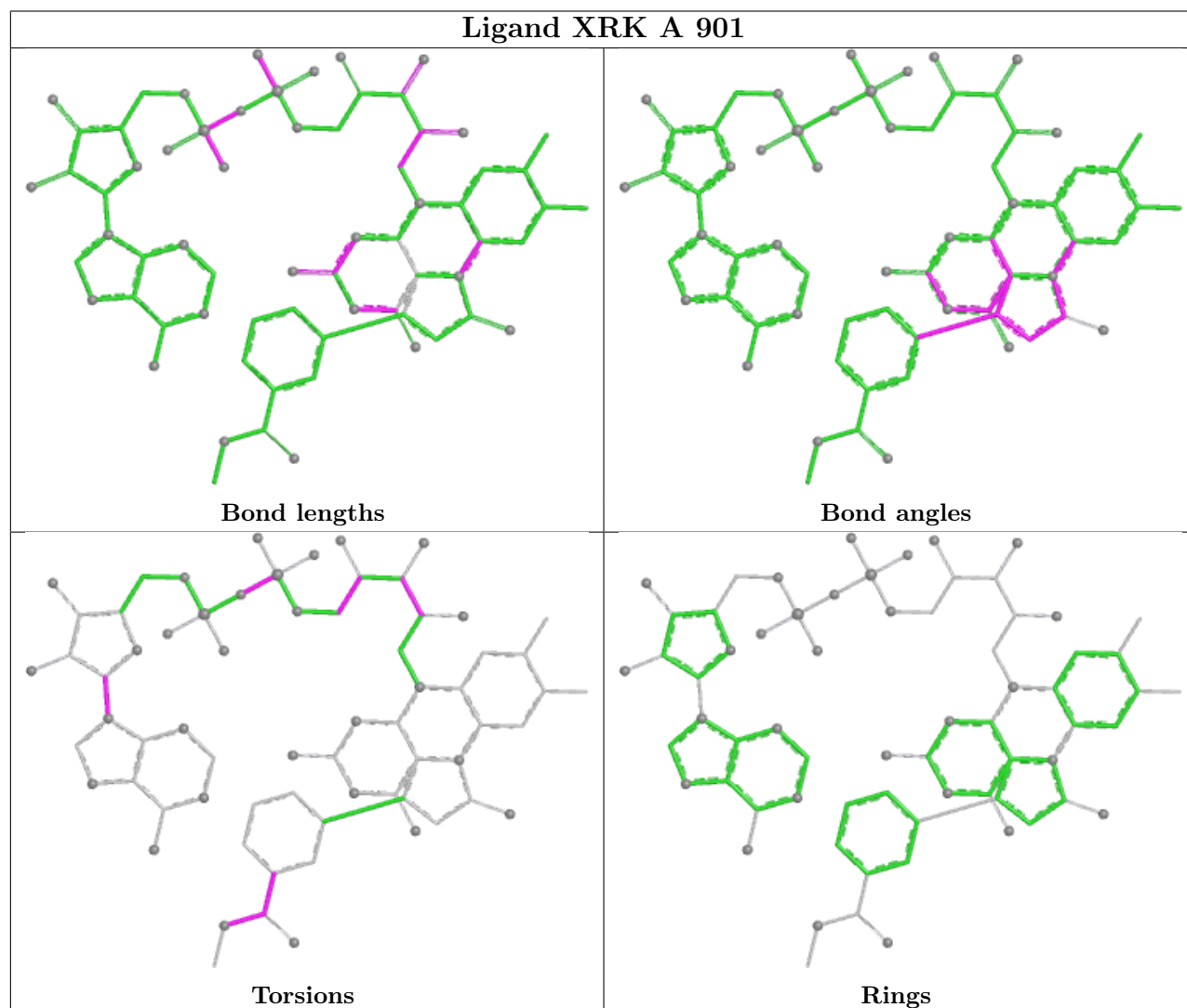
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	XRK	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	666/871 (76%)	0.43	34 (5%) 33 25	50, 82, 114, 134	0
2	B	133/144 (92%)	1.22	27 (20%) 3 2	80, 114, 139, 145	0
All	All	799/1015 (78%)	0.56	61 (7%) 20 14	50, 87, 124, 145	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	7.0
2	B	315	PHE	5.0
1	A	835	THR	4.3
1	A	667	ASP	4.2
2	B	376	ILE	4.1
1	A	171	PRO	4.0
2	B	427	ARG	3.7
1	A	518	ASP	3.4
2	B	308	ARG	3.4
2	B	440	GLU	3.3
1	A	833	MET	3.3
2	B	313	GLY	3.1
2	B	428	PHE	3.1
2	B	432	GLU	3.1
1	A	511	LEU	3.0
1	A	467	GLU	3.0
2	B	381	ALA	2.9
2	B	318	GLN	2.8
1	A	509	GLN	2.8
2	B	426	ARG	2.8
2	B	375	VAL	2.8
1	A	556	ASP	2.7
2	B	399	GLY	2.7
1	A	272	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	358	GLN	2.7
1	A	834	TYR	2.7
1	A	443	GLU	2.7
2	B	336	ARG	2.6
1	A	268	LYS	2.6
2	B	371	ARG	2.6
1	A	356	ILE	2.6
2	B	424	TYR	2.6
2	B	414	VAL	2.6
1	A	683	SER	2.5
2	B	378	LYS	2.5
1	A	786	ILE	2.4
1	A	375	ASP	2.4
1	A	274	PRO	2.4
2	B	415	VAL	2.4
2	B	323	ALA	2.3
1	A	273	LEU	2.3
2	B	379	CYS	2.3
1	A	668	ARG	2.2
2	B	347	ARG	2.2
1	A	373	GLU	2.2
1	A	269	ARG	2.2
1	A	739	ALA	2.2
1	A	271	LYS	2.2
1	A	611	SER	2.2
1	A	440	GLU	2.2
1	A	438	GLN	2.1
2	B	340	MET	2.1
1	A	508	LEU	2.1
2	B	329	THR	2.1
1	A	453	GLU	2.1
1	A	275	THR	2.1
1	A	436	LYS	2.0
1	A	492	LYS	2.0
2	B	382	ARG	2.0
2	B	411	ASN	2.0
2	B	319	GLU	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 [i](#)

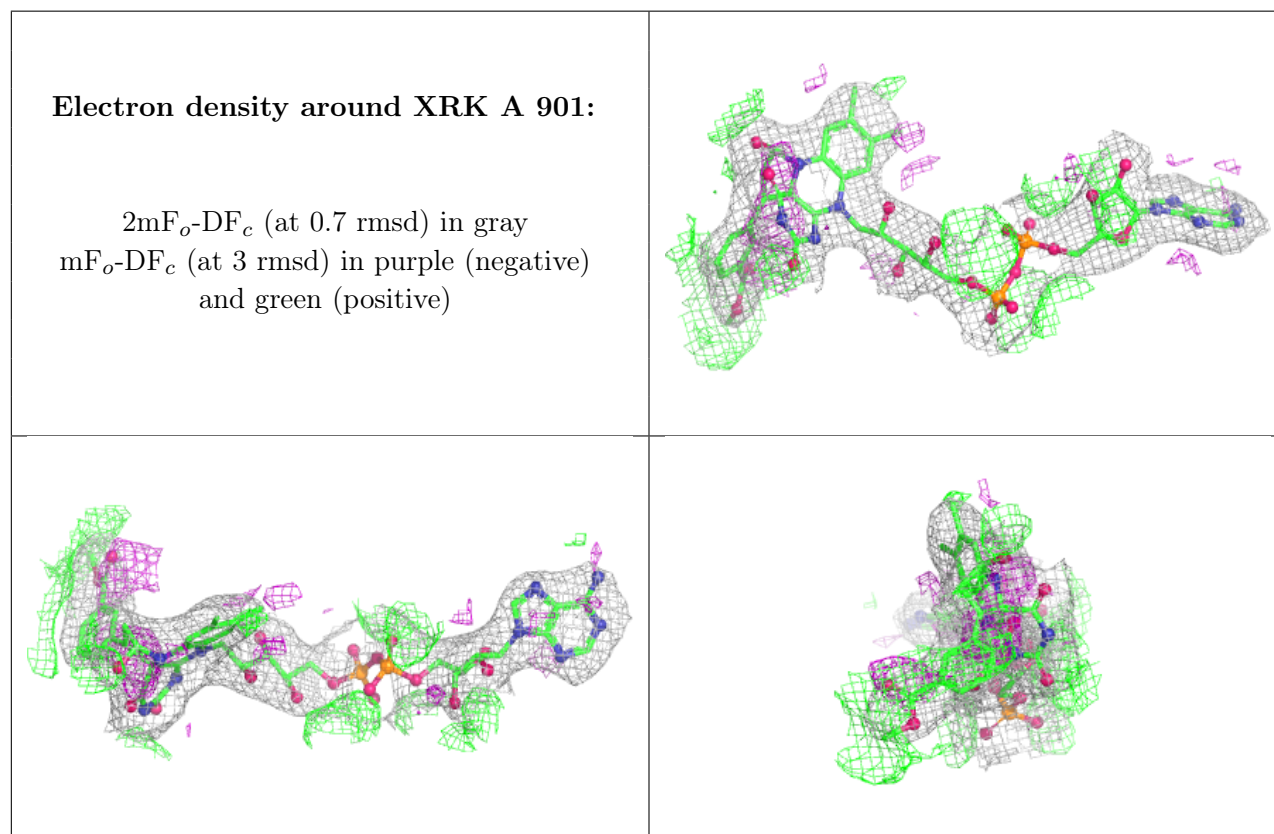
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	XRK	A	901	67/67	0.94	0.12	43,62,86,94	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.