



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:47 AM UTC

PDB ID : 6EZQ / pdb_00006ezq
Title : human Serum Albumin complexed with NBD-C12 fatty acid
Authors : Wenskowsky, L.; Liesum, A.; Schreuder, H.A.
Deposited on : 2017-11-16
Resolution : 2.39 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

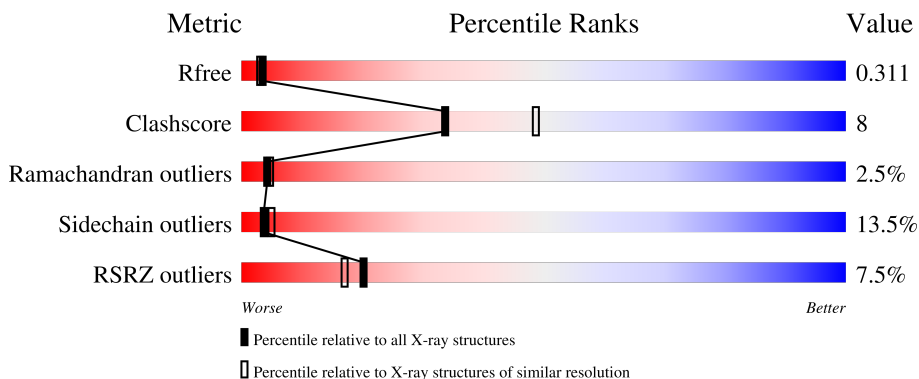
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	585	7% 65% 26% 5%

2 Entry composition [i](#)

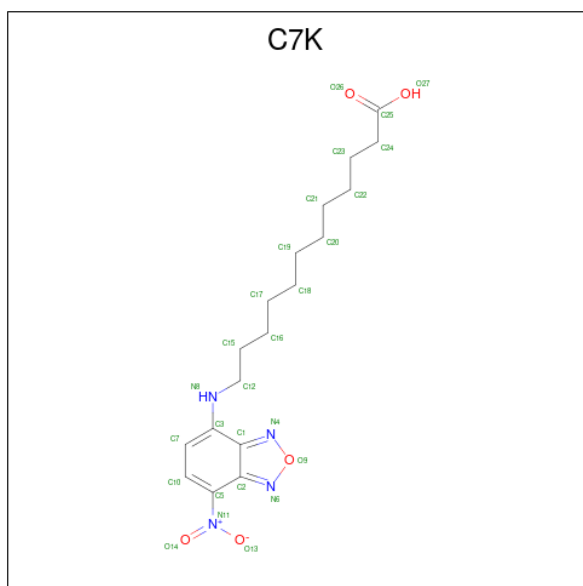
There are 3 unique types of molecules in this entry. The entry contains 4804 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4426	2794	753	838	41			

- Molecule 2 is 12-[(4-nitro-2,1,3-benzoxadiazol-7-yl)amino]dodecanoic acid (CCD ID: C7K) (formula: C₁₈H₂₆N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	18	4	5		
2	A	1	Total	C	N	O	0	0
			27	18	4	5		

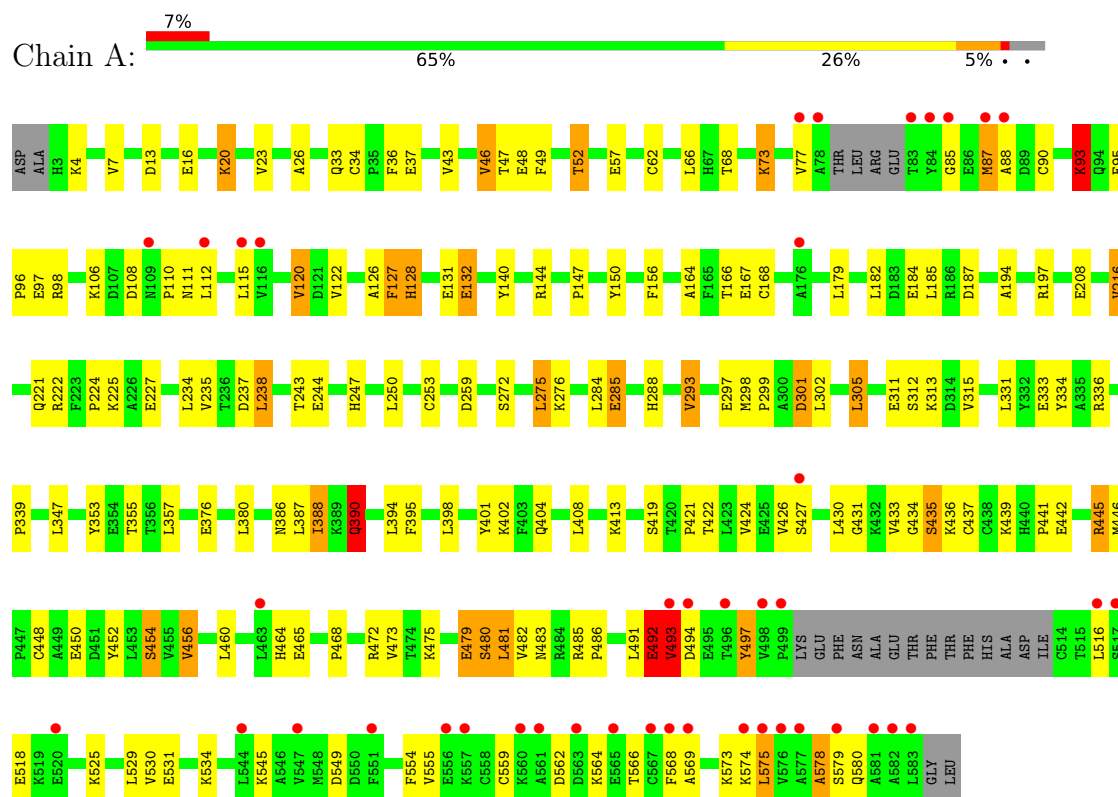
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	324	Total	O	0	0
			324	324		

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: Serum albumin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.48Å 52.72Å 123.30Å 90.00° 110.10° 90.00°	Depositor
Resolution (Å)	115.79 – 2.39 115.79 – 2.39	Depositor EDS
% Data completeness (in resolution range)	55.1 (115.79-2.39) 55.3 (115.79-2.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.182 , 0.298 0.188 , 0.311	Depositor DCC
R_{free} test set	611 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 69.9	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	0.94	EDS
Total number of atoms	4804	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% 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: C7K

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	0.89	0/4509	1.61	55/6085 (0.9%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	GLU	CA-C-N	9.11	138.36	121.97
1	A	492	GLU	C-N-CA	9.11	138.36	121.97
1	A	480	SER	CA-C-N	9.05	135.59	121.19
1	A	480	SER	C-N-CA	9.05	135.59	121.19
1	A	126	ALA	N-CA-C	-7.87	102.01	111.69
1	A	578	ALA	N-CA-C	-7.50	105.04	114.56
1	A	301	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	493	VAL	N-CA-CB	6.39	121.77	111.23
1	A	413	LYS	CA-C-N	6.33	129.28	120.29
1	A	413	LYS	C-N-CA	6.33	129.28	120.29
1	A	184	GLU	CA-C-N	6.31	128.74	120.28
1	A	184	GLU	C-N-CA	6.31	128.74	120.28
1	A	288	HIS	CA-C-N	6.01	128.59	120.65
1	A	288	HIS	C-N-CA	6.01	128.59	120.65
1	A	574	LYS	N-CA-C	-5.91	105.31	113.18
1	A	127	PHE	N-CA-C	-5.91	102.90	110.53
1	A	376	GLU	CA-C-N	5.76	129.07	120.31
1	A	376	GLU	C-N-CA	5.76	129.07	120.31
1	A	237	ASP	CA-C-N	5.75	127.91	120.44
1	A	237	ASP	C-N-CA	5.75	127.91	120.44
1	A	285	GLU	CA-C-N	5.64	128.63	120.79
1	A	285	GLU	C-N-CA	5.64	128.63	120.79
1	A	579	SER	N-CA-C	-5.63	105.19	112.68
1	A	87	MET	N-CA-C	-5.55	106.30	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	CYS	CA-C-N	5.47	128.16	120.28
1	A	62	CYS	C-N-CA	5.47	128.16	120.28
1	A	122	VAL	CA-C-N	5.47	127.87	120.44
1	A	122	VAL	C-N-CA	5.47	127.87	120.44
1	A	433	VAL	N-CA-C	-5.41	105.26	110.72
1	A	36	PHE	CA-C-N	5.40	128.27	120.38
1	A	36	PHE	C-N-CA	5.40	128.27	120.38
1	A	128	HIS	CA-C-N	5.32	127.67	120.65
1	A	128	HIS	C-N-CA	5.32	127.67	120.65
1	A	445	ARG	N-CA-C	5.32	117.51	111.02
1	A	16	GLU	CA-C-N	5.30	127.33	120.44
1	A	16	GLU	C-N-CA	5.30	127.33	120.44
1	A	96	PRO	CA-C-N	5.26	127.32	120.28
1	A	96	PRO	C-N-CA	5.26	127.32	120.28
1	A	208	GLU	CA-C-N	5.23	127.29	120.28
1	A	208	GLU	C-N-CA	5.23	127.29	120.28
1	A	401	TYR	CA-C-N	5.23	127.54	120.38
1	A	401	TYR	C-N-CA	5.23	127.54	120.38
1	A	20	LYS	CA-C-N	5.21	127.53	120.65
1	A	20	LYS	C-N-CA	5.21	127.53	120.65
1	A	93	LYS	CA-C-N	5.18	129.72	122.36
1	A	93	LYS	C-N-CA	5.18	129.72	122.36
1	A	187	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	194	ALA	CA-C-N	5.12	127.65	120.28
1	A	194	ALA	C-N-CA	5.12	127.65	120.28
1	A	259	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	452	TYR	N-CA-C	-5.06	107.66	113.88
1	A	187	ASP	CA-C-N	5.02	127.51	120.28
1	A	187	ASP	C-N-CA	5.02	127.51	120.28
1	A	473	VAL	CA-C-N	5.01	127.69	120.38
1	A	473	VAL	C-N-CA	5.01	127.69	120.38

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	4426	0	4334	68	0
2	A	54	0	0	0	0
3	A	324	0	0	2	0
All	All	4804	0	4334	68	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 8.

All (68) 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:112:LEU:HD22	1:A:144:ARG:HH21	1.35	0.92
1:A:493:VAL:HG23	1:A:494:ASP:N	2.03	0.73
1:A:408:LEU:HD22	1:A:530:VAL:HG22	1.72	0.69
1:A:492:GLU:O	1:A:493:VAL:HG13	1.95	0.67
1:A:112:LEU:HD22	1:A:144:ARG:NH2	2.09	0.63
1:A:305:LEU:HD11	1:A:333:GLU:HB3	1.80	0.63
1:A:49:PHE:O	1:A:52:THR:HB	2.00	0.62
1:A:140:TYR:CZ	1:A:144:ARG:HD2	2.35	0.61
1:A:493:VAL:HG23	1:A:494:ASP:H	1.65	0.61
1:A:422:THR:O	1:A:426:VAL:HG23	2.02	0.59
1:A:404:GLN:HE21	1:A:431:GLY:HA3	1.68	0.58
1:A:427:SER:HA	1:A:430:LEU:HD12	1.85	0.58
1:A:450:GLU:O	1:A:454:SER:HB2	2.03	0.58
1:A:353:TYR:CE2	1:A:357:LEU:HD11	2.39	0.57
1:A:481:LEU:H	1:A:481:LEU:HD23	1.70	0.56
1:A:421:PRO:HA	1:A:424:VAL:HG12	1.88	0.56
1:A:222:ARG:HD3	1:A:293:VAL:HG12	1.87	0.56
1:A:46:VAL:HG13	1:A:73:LYS:HD3	1.88	0.56
1:A:234:LEU:O	1:A:238:LEU:HB2	2.05	0.55
1:A:305:LEU:HD21	1:A:334:TYR:HA	1.89	0.54
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.74	0.53
1:A:90:CYS:O	1:A:98:ARG:HG3	2.08	0.53
1:A:426:VAL:HA	1:A:456:VAL:HG21	1.90	0.53
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.91	0.53
1:A:437:CYS:O	1:A:445:ARG:HG2	2.09	0.52
1:A:331:LEU:HD11	1:A:347:LEU:HD21	1.93	0.50
1:A:216:VAL:HG23	1:A:235:VAL:HG21	1.93	0.50
1:A:394:LEU:HG	1:A:398:LEU:HD12	1.93	0.49
1:A:408:LEU:HD22	1:A:530:VAL:CG2	2.40	0.49
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.95	0.49
1:A:398:LEU:HB3	1:A:402:LYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:PHE:CD1	1:A:434:GLY:HA3	2.48	0.48
1:A:221:GLN:HG2	1:A:339:PRO:HA	1.95	0.47
1:A:472:ARG:HH12	1:A:497:TYR:HE2	1.61	0.46
1:A:224:PRO:HB2	1:A:298:MET:HA	1.97	0.46
1:A:108:ASP:O	1:A:110:PRO:HD3	2.15	0.45
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.99	0.45
1:A:20:LYS:HG2	1:A:47:THR:HG21	1.99	0.45
1:A:386:ASN:O	1:A:390:GLN:HB2	2.17	0.45
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.98	0.45
1:A:441:PRO:O	1:A:445:ARG:HG3	2.16	0.45
1:A:388:ILE:HD13	1:A:446:MET:HG3	1.98	0.44
1:A:475:LYS:O	1:A:479:GLU:HB2	2.16	0.44
1:A:93:LYS:HB3	1:A:97:GLU:HB3	2.00	0.44
1:A:164:ALA:O	1:A:168:CYS:HB2	2.18	0.44
1:A:331:LEU:HD11	1:A:347:LEU:CD2	2.47	0.44
1:A:276:LYS:HA	3:A:760:HOH:O	2.17	0.43
1:A:559:CYS:SG	1:A:568:PHE:HZ	2.41	0.43
1:A:445:ARG:O	1:A:448:CYS:HB3	2.18	0.43
1:A:575:LEU:HA	1:A:578:ALA:HB3	1.99	0.43
1:A:68:THR:HA	1:A:98:ARG:HH22	1.83	0.43
1:A:464:HIS:CD2	1:A:468:PRO:HA	2.54	0.43
1:A:243:THR:O	1:A:247:HIS:HD2	2.00	0.43
1:A:85:GLY:H	1:A:88:ALA:HB2	1.84	0.42
1:A:569:ALA:HA	3:A:856:HOH:O	2.20	0.42
1:A:156:PHE:HB2	1:A:284:LEU:HB3	2.02	0.42
1:A:426:VAL:HG21	1:A:460:LEU:HD12	2.01	0.42
1:A:353:TYR:CZ	1:A:357:LEU:HD11	2.54	0.41
1:A:481:LEU:HG	1:A:482:VAL:H	1.85	0.41
1:A:224:PRO:HB3	1:A:336:ARG:HB2	2.03	0.41
1:A:312:SER:HB3	1:A:315:VAL:HG23	2.03	0.41
1:A:426:VAL:HG22	1:A:456:VAL:HG22	2.01	0.41
1:A:483:ASN:C	1:A:486:PRO:HD2	2.44	0.41
1:A:531:GLU:O	1:A:534:LYS:HB2	2.19	0.41
1:A:127:PHE:O	1:A:128:HIS:HB2	2.21	0.41
1:A:244:GLU:HB2	1:A:253:CYS:HB3	2.03	0.41
1:A:225:LYS:HA	1:A:299:PRO:HG3	2.03	0.41
1:A:272:SER:HB3	1:A:275:LEU:CD1	2.51	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	557/585 (95%)	488 (88%)	55 (10%)	14 (2%)	4 5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	493	VAL
1	A	492	GLU
1	A	4	LYS
1	A	93	LYS
1	A	150	TYR
1	A	479	GLU
1	A	120	VAL
1	A	132	GLU
1	A	390	GLN
1	A	435	SER
1	A	77	VAL
1	A	95	GLU
1	A	302	LEU
1	A	564	LYS

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	482/511 (94%)	417 (86%)	65 (14%)	4 5

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	13	ASP
1	A	33	GLN
1	A	34	CYS
1	A	37	GLU
1	A	46	VAL
1	A	48	GLU
1	A	52	THR
1	A	57	GLU
1	A	66	LEU
1	A	73	LYS
1	A	87	MET
1	A	111	ASN
1	A	115	LEU
1	A	120	VAL
1	A	131	GLU
1	A	132	GLU
1	A	166	THR
1	A	167	GLU
1	A	179	LEU
1	A	182	LEU
1	A	185	LEU
1	A	197	ARG
1	A	216	VAL
1	A	227	GLU
1	A	238	LEU
1	A	275	LEU
1	A	293	VAL
1	A	297	GLU
1	A	301	ASP
1	A	305	LEU
1	A	311	GLU
1	A	313	LYS
1	A	355	THR
1	A	380	LEU
1	A	387	LEU
1	A	388	ILE
1	A	390	GLN
1	A	419	SER
1	A	435	SER
1	A	436	LYS
1	A	439	LYS
1	A	442	GLU

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Mol	Chain	Res	Type
1	A	454	SER
1	A	456	VAL
1	A	465	GLU
1	A	480	SER
1	A	481	LEU
1	A	485	ARG
1	A	491	LEU
1	A	493	VAL
1	A	497	TYR
1	A	516	LEU
1	A	518	GLU
1	A	525	LYS
1	A	529	LEU
1	A	545	LYS
1	A	549	ASP
1	A	554	PHE
1	A	555	VAL
1	A	562	ASP
1	A	566	THR
1	A	573	LYS
1	A	575	LEU
1	A	580	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	61	ASN
1	A	111	ASN
1	A	221	GLN
1	A	247	HIS
1	A	318	ASN
1	A	367	HIS
1	A	404	GLN
1	A	459	GLN
1	A	526	GLN
1	A	535	HIS
1	A	580	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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
2	C7K	A	601	-	28,28,28	1.31	4 (14%)	27,35,35	1.54	5 (18%)
2	C7K	A	602	-	28,28,28	1.11	3 (10%)	27,35,35	1.17	3 (11%)

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
2	C7K	A	601	-	-	8/17/19/19	0/2/2/2
2	C7K	A	602	-	-	7/17/19/19	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	C7K	C1-N4	3.40	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	C7K	C2-N6	3.16	1.36	1.31
2	A	602	C7K	O9-N4	-2.74	1.33	1.39
2	A	602	C7K	O26-C25	2.74	1.31	1.22
2	A	601	C7K	O26-C25	2.68	1.30	1.22
2	A	602	C7K	O27-C25	-2.68	1.22	1.30
2	A	601	C7K	O27-C25	-2.53	1.22	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	C7K	C1-C3-N8	3.98	122.38	117.92
2	A	601	C7K	O9-N4-C1	3.26	109.55	105.65
2	A	601	C7K	O26-C25-C24	-3.23	112.85	123.09
2	A	601	C7K	O27-C25-C24	3.05	123.65	114.00
2	A	602	C7K	O26-C25-C24	-3.00	113.57	123.09
2	A	602	C7K	O27-C25-C24	2.80	122.84	114.00
2	A	602	C7K	C1-C3-N8	-2.39	115.25	117.92
2	A	601	C7K	C12-N8-C3	2.24	128.78	123.35

There are no chirality outliers.

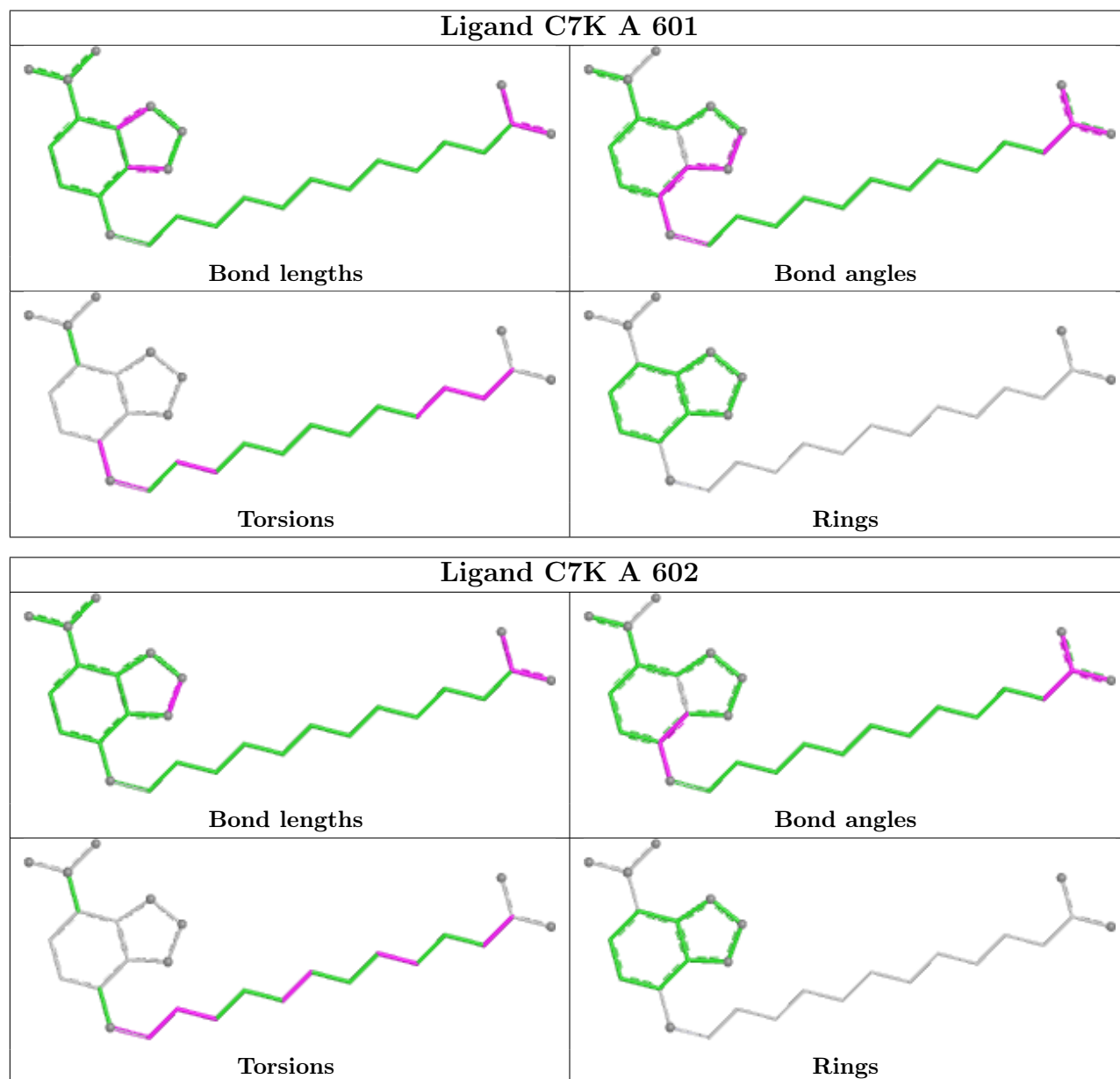
All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	C7K	C1-C3-N8-C12
2	A	601	C7K	C7-C3-N8-C12
2	A	601	C7K	C22-C23-C24-C25
2	A	602	C7K	C20-C21-C22-C23
2	A	602	C7K	C12-C15-C16-C17
2	A	601	C7K	C15-C12-N8-C3
2	A	602	C7K	C17-C18-C19-C20
2	A	601	C7K	C12-C15-C16-C17
2	A	602	C7K	C15-C12-N8-C3
2	A	602	C7K	N8-C12-C15-C16
2	A	602	C7K	C23-C24-C25-O26
2	A	601	C7K	C23-C24-C25-O26
2	A	602	C7K	C23-C24-C25-O27
2	A	601	C7K	C23-C24-C25-O27
2	A	601	C7K	C21-C22-C23-C24

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	563/585 (96%)	0.53	42 (7%) 20 17	18, 47, 92, 114	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	561	ALA	5.0
1	A	557	LYS	4.9
1	A	516	LEU	4.7
1	A	499	PRO	4.1
1	A	517	SER	3.7
1	A	493	VAL	3.4
1	A	576	VAL	3.4
1	A	498	VAL	3.3
1	A	83	THR	3.2
1	A	581	ALA	3.0
1	A	87	MET	2.9
1	A	583	LEU	2.9
1	A	579	SER	2.8
1	A	77	VAL	2.8
1	A	109	ASN	2.7
1	A	582	ALA	2.7
1	A	577	ALA	2.6
1	A	463	LEU	2.6
1	A	78	ALA	2.6
1	A	569	ALA	2.6
1	A	116	VAL	2.5
1	A	494	ASP	2.5
1	A	496	THR	2.4
1	A	563	ASP	2.4
1	A	544	LEU	2.4
1	A	520	GLU	2.4
1	A	567	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	551	PHE	2.3
1	A	176	ALA	2.3
1	A	547	VAL	2.3
1	A	112	LEU	2.2
1	A	556	GLU	2.2
1	A	88	ALA	2.2
1	A	84	TYR	2.2
1	A	115	LEU	2.2
1	A	568	PHE	2.2
1	A	560	LYS	2.1
1	A	574	LYS	2.1
1	A	427	SER	2.1
1	A	565	GLU	2.1
1	A	575	LEU	2.0
1	A	85	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

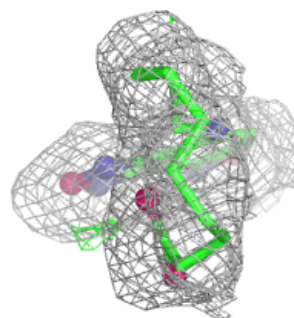
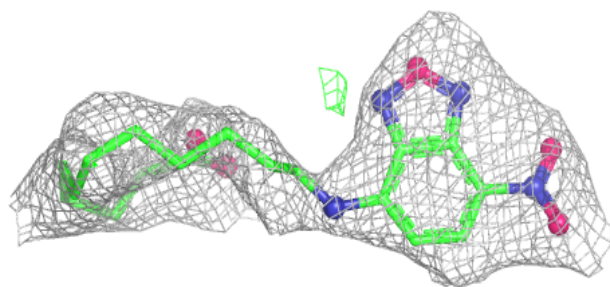
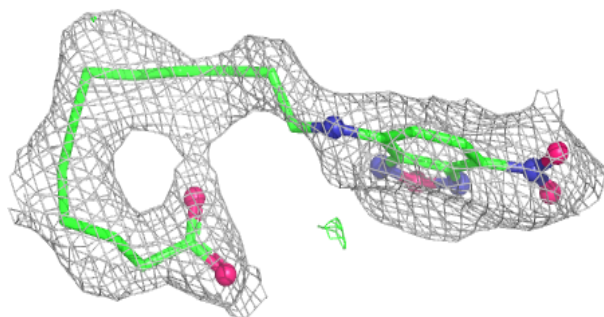
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C7K	A	601	27/27	0.86	0.12	43,53,60,60	0
2	C7K	A	602	27/27	0.87	0.13	32,39,41,42	27

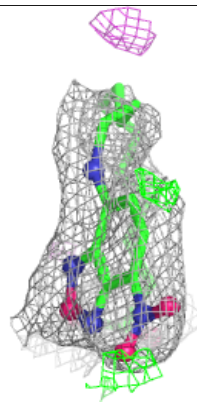
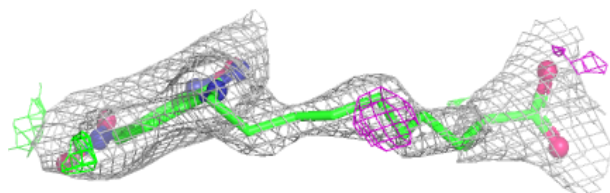
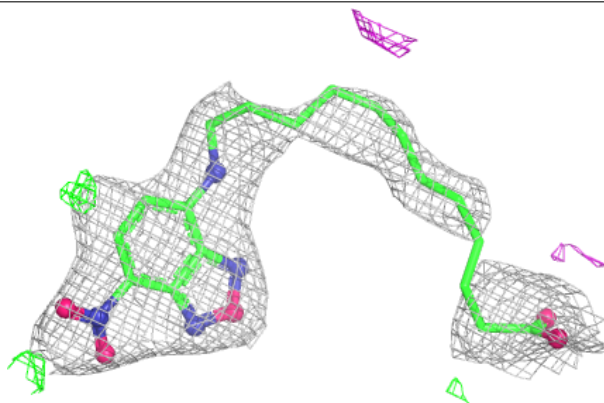
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around C7K A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around C7K A 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.