Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:46 AM UTC

PDB ID	:	6GNJ / pdb_00006gnj
Title	:	Exoenzyme S from Pseudomonas aeruginosa in complex with human 14-3-3 protein beta, trimeric crystal form in complex with STO1101
Authors	:	Karlberg, T.; Pinto, A.F.; Hornyak, P.; Thorsell, A.G.; Nareoja, K.; Schuler, H.
Deposited on	:	2018-05-31
Resolution	:	3.24 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:

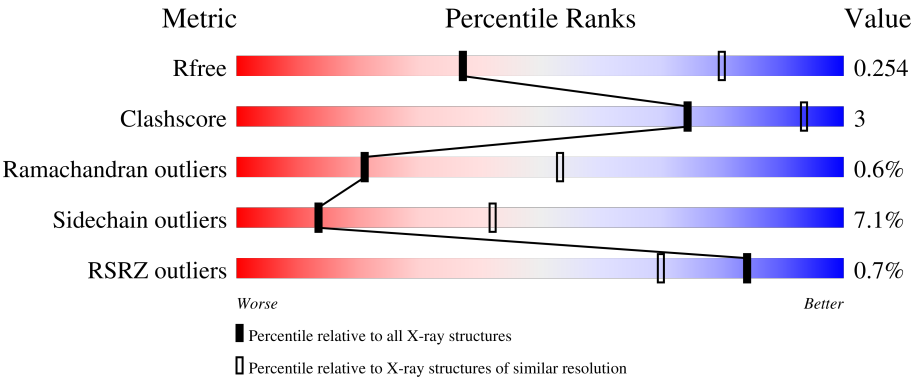
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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 <=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	243	83% 12% • 5%
1	B	243	% 79% 15% 5%
2	C	244	% 65% 19% • 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5298 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 14-3-3 protein beta/alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1864	1166	313	376	9			
1	B	230	Total	C	N	O	S	0	0	0
			1855	1161	312	373	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP P31946
A	236	ASN	-	expression tag	UNP P31946
A	237	LEU	-	expression tag	UNP P31946
A	238	TYR	-	expression tag	UNP P31946
A	239	PHE	-	expression tag	UNP P31946
A	240	GLN	-	expression tag	UNP P31946
A	241	SER	-	expression tag	UNP P31946
A	242	LEU	-	expression tag	UNP P31946
A	243	GLU	-	expression tag	UNP P31946
B	235	GLU	-	expression tag	UNP P31946
B	236	ASN	-	expression tag	UNP P31946
B	237	LEU	-	expression tag	UNP P31946
B	238	TYR	-	expression tag	UNP P31946
B	239	PHE	-	expression tag	UNP P31946
B	240	GLN	-	expression tag	UNP P31946
B	241	SER	-	expression tag	UNP P31946
B	242	LEU	-	expression tag	UNP P31946
B	243	GLU	-	expression tag	UNP P31946

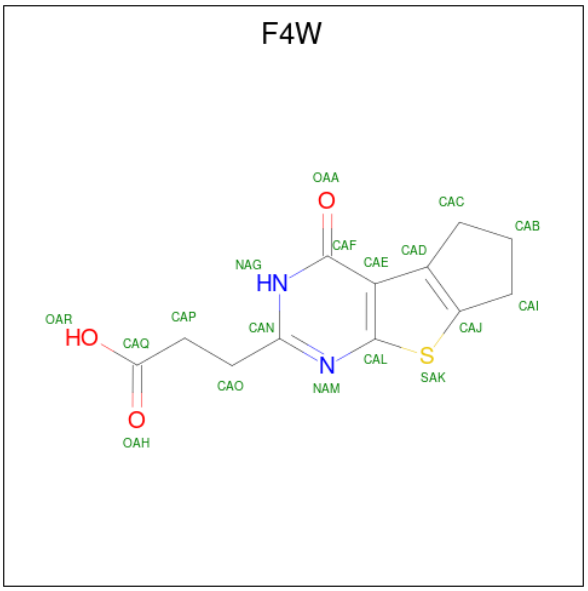
- Molecule 2 is a protein called Exoenzyme S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	210	Total	C	N	O	S	0	0	0
			1561	962	284	311	4			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	210	MET	-	initiating methionine	UNP Q93SQ1
C	211	GLY	-	expression tag	UNP Q93SQ1
C	212	SER	-	expression tag	UNP Q93SQ1
C	213	SER	-	expression tag	UNP Q93SQ1
C	214	HIS	-	expression tag	UNP Q93SQ1
C	215	HIS	-	expression tag	UNP Q93SQ1
C	216	HIS	-	expression tag	UNP Q93SQ1
C	217	HIS	-	expression tag	UNP Q93SQ1
C	218	HIS	-	expression tag	UNP Q93SQ1
C	219	HIS	-	expression tag	UNP Q93SQ1
C	220	SER	-	expression tag	UNP Q93SQ1
C	221	GLN	-	expression tag	UNP Q93SQ1
C	222	ASP	-	expression tag	UNP Q93SQ1
C	223	PRO	-	expression tag	UNP Q93SQ1
C	224	ASN	-	expression tag	UNP Q93SQ1
C	225	SER	-	expression tag	UNP Q93SQ1
C	226	GLU	-	expression tag	UNP Q93SQ1
C	227	ASN	-	expression tag	UNP Q93SQ1
C	228	LEU	-	expression tag	UNP Q93SQ1
C	229	TYR	-	expression tag	UNP Q93SQ1
C	230	PHE	-	expression tag	UNP Q93SQ1
C	231	GLN	-	expression tag	UNP Q93SQ1
C	232	GLY	-	expression tag	UNP Q93SQ1
C	379	ALA	GLU	engineered mutation	UNP Q93SQ1
C	381	ALA	GLU	engineered mutation	UNP Q93SQ1

- Molecule 3 is 3-(12-oxidanylidene-7-thia-9,11-diazatricyclo[6.4.0.0^{2,6}]dodeca-1(8),2(6),9-trien-10-yl)propanoic acid (CCD ID: F4W) (formula: $C_{12}H_{12}N_2O_3S$).



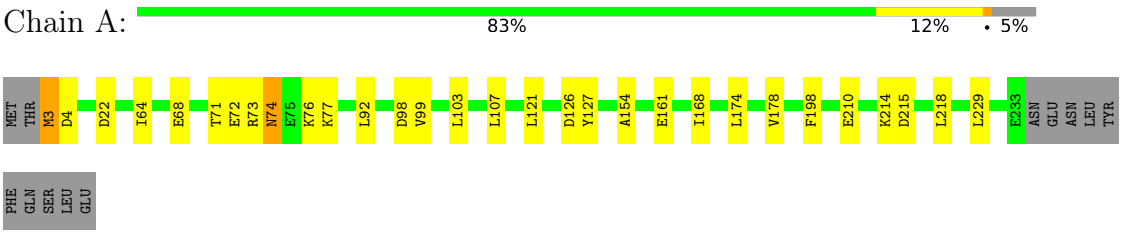
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			18	12	2	3	1		

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.

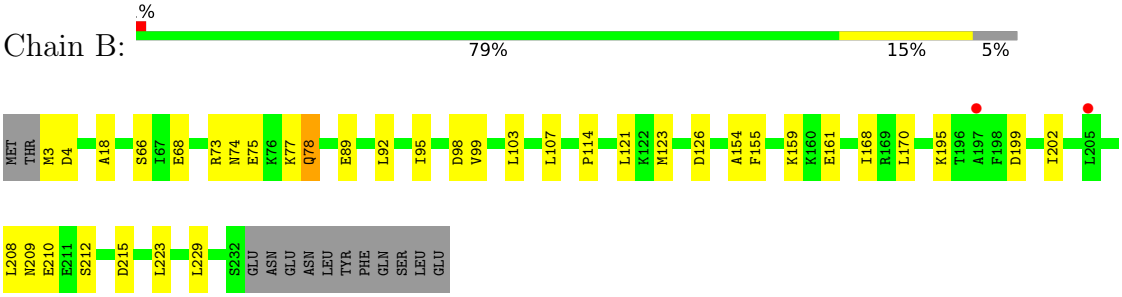
• Molecule 1: 14-3-3 protein beta/alpha

Chain A:



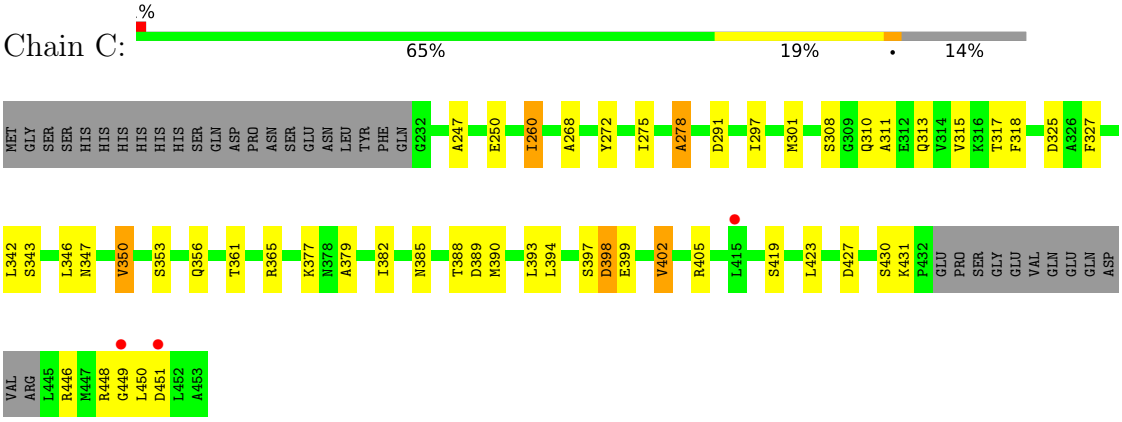
• Molecule 1: 14-3-3 protein beta/alpha

Chain B:



• Molecule 2: Exoenzyme S

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	160.40Å 59.36Å 120.64Å 90.00° 125.84° 90.00°	Depositor
Resolution (Å)	48.90 – 3.24 48.90 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.90-3.24) 99.2 (48.90-3.24)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.173 , 0.221 0.201 , 0.254	Depositor DCC
R_{free} test set	1037 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å^2)	89.8	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 84.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5298	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: F4W

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	0/1891	1.52	11/2545 (0.4%)
1	B	0.87	0/1882	1.53	12/2533 (0.5%)
2	C	0.91	0/1578	1.49	14/2117 (0.7%)
All	All	0.89	0/5351	1.52	37/7195 (0.5%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	427	ASP	CA-CB-CG	12.09	124.69	112.60
1	A	3	MET	CA-C-N	8.20	133.81	120.94
1	A	3	MET	C-N-CA	8.20	133.81	120.94
2	C	291	ASP	CA-CB-CG	6.73	119.33	112.60
1	A	4	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	98	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	74	ASN	CA-C-N	6.42	129.76	120.38
1	A	74	ASN	C-N-CA	6.42	129.76	120.38
1	B	98	ASP	CA-CB-CG	6.30	118.90	112.60
2	C	389	ASP	CA-CB-CG	6.02	118.62	112.60
2	C	278	ALA	CA-C-N	5.88	128.44	120.38
2	C	278	ALA	C-N-CA	5.88	128.44	120.38
2	C	451	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	126	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	4	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	114	PRO	CA-C-N	5.52	127.94	120.38
1	B	114	PRO	C-N-CA	5.52	127.94	120.38
1	A	22	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	215	ASP	CA-CB-CG	5.44	118.04	112.60
2	C	385	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	198	PHE	CA-C-N	5.25	127.57	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	PHE	C-N-CA	5.25	127.57	120.38
1	A	126	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	170	LEU	CA-C-N	5.17	125.72	119.98
1	B	170	LEU	C-N-CA	5.17	125.72	119.98
2	C	399	GLU	N-CA-C	-5.16	106.81	113.01
2	C	377	LYS	CA-C-N	5.15	130.25	122.68
2	C	377	LYS	C-N-CA	5.15	130.25	122.68
2	C	272	TYR	CA-C-N	5.12	127.39	120.38
2	C	272	TYR	C-N-CA	5.12	127.39	120.38
1	A	215	ASP	CA-CB-CG	5.11	117.70	112.60
2	C	268	ALA	CA-C-N	5.09	127.10	120.28
2	C	268	ALA	C-N-CA	5.09	127.10	120.28
1	B	195	LYS	CA-C-N	5.08	127.39	120.54
1	B	195	LYS	C-N-CA	5.08	127.39	120.54
1	B	89	GLU	CA-C-N	5.02	126.96	120.44
1	B	89	GLU	C-N-CA	5.02	126.96	120.44

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	1864	0	1841	11	0
1	B	1855	0	1835	10	0
2	C	1561	0	1542	15	0
3	C	18	0	0	0	0
All	All	5298	0	5218	33	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 3.

All (33) 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:B:103:LEU:HD21	1:B:123:MET:HE2	1.72	0.71
1:A:99:VAL:HG11	1:A:127:TYR:CD2	2.26	0.70
1:A:74:ASN:HB3	1:A:77:LYS:HB2	1.77	0.66
1:A:64:ILE:HD11	1:B:18:ALA:HB2	1.78	0.65
2:C:247:ALA:HA	2:C:250:GLU:HB2	1.84	0.59
1:A:218:LEU:HD22	2:C:423:LEU:HD21	1.85	0.58
2:C:325:ASP:HB3	2:C:405:ARG:HH22	1.67	0.58
1:B:209:ASN:HB3	1:B:212:SER:HB3	1.88	0.56
2:C:260:ILE:H	2:C:260:ILE:HD12	1.71	0.56
2:C:327:PHE:CE1	2:C:390:MET:HB2	2.41	0.56
1:B:74:ASN:HB3	1:B:77:LYS:HB2	1.89	0.55
2:C:297:ILE:HG22	2:C:301:MET:HE2	1.89	0.54
1:A:72:GLU:H	1:A:73:ARG:NH1	2.06	0.53
1:B:103:LEU:HA	1:B:107:LEU:HB2	1.92	0.51
1:A:103:LEU:HA	1:A:107:LEU:HB2	1.92	0.51
1:B:199:ASP:HA	1:B:202:ILE:HG12	1.92	0.51
1:B:121:LEU:HB3	1:B:154:ALA:HB2	1.92	0.50
1:A:121:LEU:HB3	1:A:154:ALA:HB2	1.92	0.50
1:A:174:LEU:O	1:A:178:VAL:HG23	2.13	0.48
1:A:214:LYS:HG3	2:C:393:LEU:HD13	1.94	0.48
2:C:350:VAL:HG11	2:C:379:ALA:HA	1.95	0.48
2:C:448:ARG:HG3	2:C:449:GLY:H	1.80	0.47
2:C:327:PHE:HE1	2:C:390:MET:HB2	1.80	0.47
2:C:398:ASP:HB2	2:C:402:VAL:O	2.16	0.46
1:B:95:ILE:O	1:B:99:VAL:HG23	2.16	0.46
1:A:72:GLU:H	1:A:73:ARG:HH12	1.63	0.46
2:C:317:THR:HG21	2:C:382:ILE:HB	1.98	0.45
2:C:318:PHE:CE1	2:C:361:THR:HG23	2.51	0.45
1:B:74:ASN:O	1:B:78:GLN:HB2	2.18	0.43
1:A:71:THR:HA	1:A:73:ARG:HH12	1.82	0.43
2:C:310:GLN:HG3	2:C:365:ARG:HB3	2.02	0.42
1:B:155:PHE:CZ	1:B:159:LYS:HE3	2.56	0.41
2:C:350:VAL:O	2:C:353:SER:HB3	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	229/243 (94%)	223 (97%)	6 (3%)	0	100 100
1	B	228/243 (94%)	217 (95%)	10 (4%)	1 (0%)	30 60
2	C	206/244 (84%)	186 (90%)	17 (8%)	3 (2%)	8 34
All	All	663/730 (91%)	626 (94%)	33 (5%)	4 (1%)	21 53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	278	ALA
1	B	210	GLU
2	C	308	SER
2	C	311	ALA

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	205/217 (94%)	197 (96%)	8 (4%)	28 58
1	B	204/217 (94%)	192 (94%)	12 (6%)	18 48
2	C	157/189 (83%)	137 (87%)	20 (13%)	4 19
All	All	566/623 (91%)	526 (93%)	40 (7%)	13 42

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	68	GLU
1	A	76	LYS
1	A	92	LEU
1	A	161	GLU

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Mol	Chain	Res	Type
1	A	168	ILE
1	A	210	GLU
1	A	229	LEU
1	B	3	MET
1	B	66	SER
1	B	68	GLU
1	B	73	ARG
1	B	75	GLU
1	B	78	GLN
1	B	92	LEU
1	B	161	GLU
1	B	168	ILE
1	B	208	LEU
1	B	223	LEU
1	B	229	LEU
2	C	260	ILE
2	C	275	ILE
2	C	313	GLN
2	C	315	VAL
2	C	342	LEU
2	C	343	SER
2	C	346	LEU
2	C	347	ASN
2	C	350	VAL
2	C	356	GLN
2	C	388	THR
2	C	394	LEU
2	C	397	SER
2	C	398	ASP
2	C	402	VAL
2	C	419	SER
2	C	430	SER
2	C	431	LYS
2	C	446	ARG
2	C	450	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	B	78	GLN
1	B	79	GLN

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Mol	Chain	Res	Type
1	B	226	ASN
2	C	286	GLN
2	C	356	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	F4W	C	501	-	18,20,20	4.13	7 (38%)	22,29,29	5.86	13 (59%)

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	F4W	C	501	-	-	2/5/11/11	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	F4W	CAJ-SAK	-12.02	1.49	1.74
3	C	501	F4W	CAL-SAK	-9.13	1.49	1.73
3	C	501	F4W	CAO-CAN	-5.46	1.40	1.49
3	C	501	F4W	CAC-CAD	-4.20	1.41	1.51
3	C	501	F4W	CAP-CAQ	2.63	1.56	1.50
3	C	501	F4W	CAE-CAD	-2.61	1.38	1.44
3	C	501	F4W	OAH-CAQ	2.15	1.29	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	F4W	CAJ-SAK-CAL	20.61	102.01	91.34
3	C	501	F4W	SAK-CAL-NAM	8.55	128.84	121.44
3	C	501	F4W	CAF-NAG-CAN	-8.39	119.05	123.90
3	C	501	F4W	CAD-CAE-CAL	-6.93	108.59	112.89
3	C	501	F4W	CAI-CAJ-SAK	5.38	142.15	128.57
3	C	501	F4W	CAE-CAL-NAM	-4.99	121.87	127.24
3	C	501	F4W	CAC-CAB-CAI	-3.98	97.21	107.18
3	C	501	F4W	CAD-CAJ-SAK	-3.73	108.92	112.43
3	C	501	F4W	CAE-CAL-SAK	-3.29	109.28	111.19
3	C	501	F4W	NAG-CAN-NAM	-3.26	118.94	123.08
3	C	501	F4W	CAB-CAI-CAJ	2.69	105.67	101.92
3	C	501	F4W	CAO-CAP-CAQ	2.53	120.38	113.67
3	C	501	F4W	OAA-CAF-NAG	-2.34	115.71	120.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	F4W	CAO-CAP-CAQ-OAH
3	C	501	F4W	CAO-CAP-CAQ-OAR

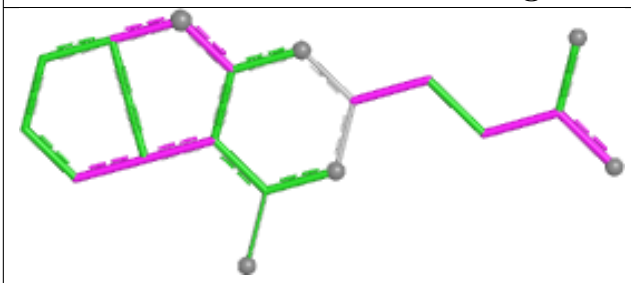
There are no ring outliers.

No monomer is involved in short contacts.

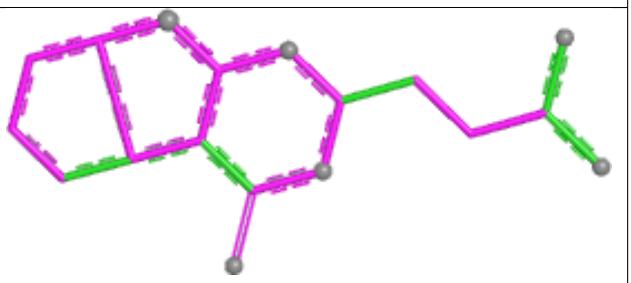
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

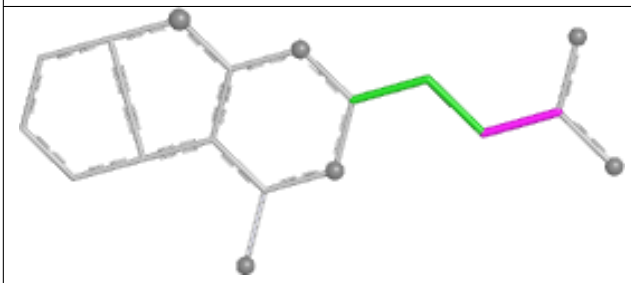
Ligand F4W C 501



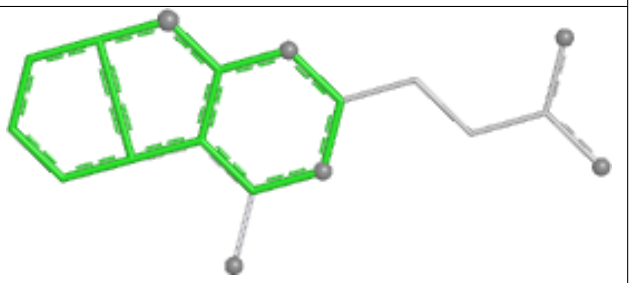
Bond lengths



Bond angles



Torsions



Rings

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	231/243 (95%)	-0.23	0	100	100	61, 82, 131, 173	0
1	B	230/243 (94%)	0.11	2 (0%)	81	64	67, 117, 195, 207	0
2	C	210/244 (86%)	-0.16	3 (1%)	73	54	64, 88, 131, 166	0
All	All	671/730 (91%)	-0.10	5 (0%)	84	70	61, 91, 173, 207	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	415	LEU	2.9
2	C	449	GLY	2.7
1	B	205	LEU	2.4
2	C	451	ASP	2.1
1	B	197	ALA	2.1

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

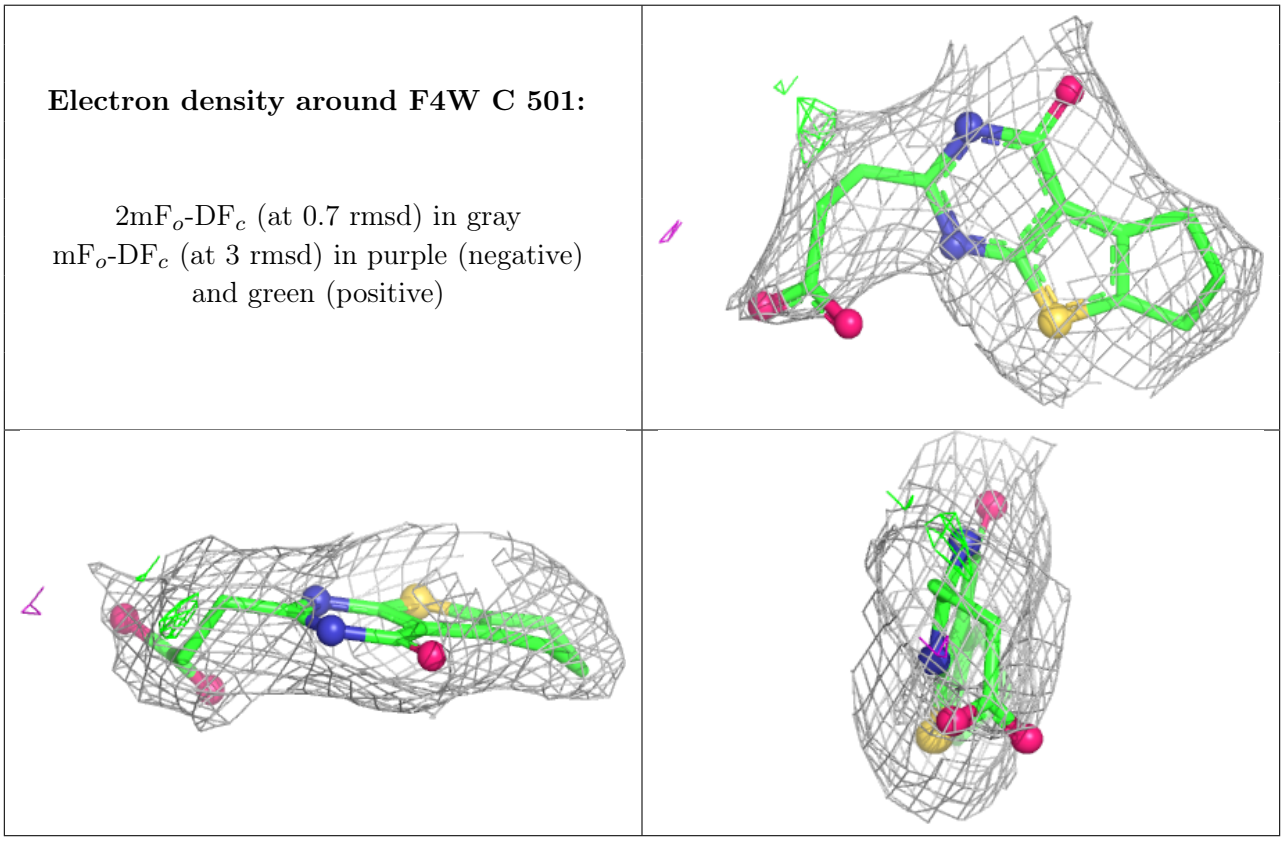
There are no oligosaccharides in this entry.

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(Å^2)	Q<0.9
3	F4W	C	501	18/18	0.94	0.11	94,102,117,119	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.