



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:02 PM UTC

PDB ID : 9FWG / pdb_00009fwg
Title : LSD1/CoREST bound to bomedemstat
Authors : Speranzini, V.; Mattevi, A.
Deposited on : 2024-06-30
Resolution : 3.20 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

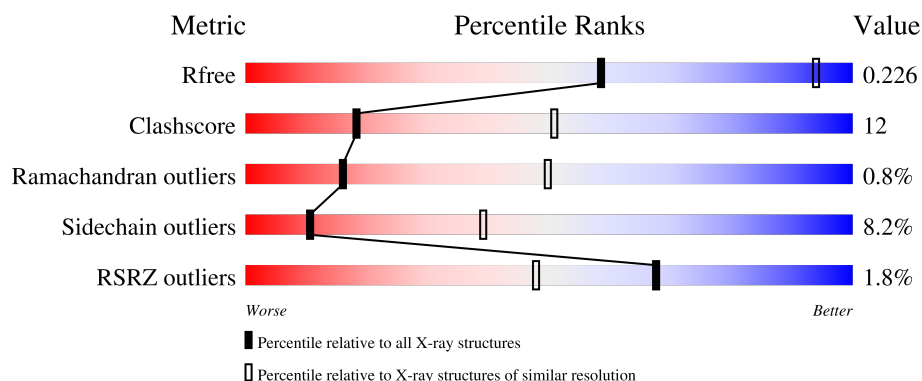
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	852	 48% 26% 22%
2	B	485	 16% 10% 73%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6357 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.

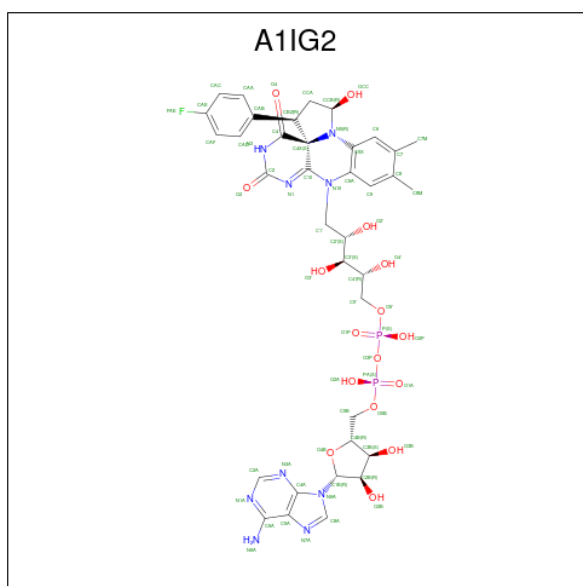
- Molecule 1 is a protein called Lysine-specific histone demethylase 1A.

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

- 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			

- Molecule 3 is Bomedemstat FAD adduct (CCD ID: A1IG2) (formula: $C_{36}H_{42}FN_9O_{16}P_2$) (labeled as "Ligand of Interest" by depositor).

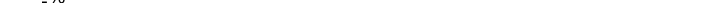


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	0	0
			64	36	1	9	16	2		

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.

- Chain A: 48% 26% 22%

Position	R805	N806	Y807	P808	A809	T810	A814	L815	S817	G818	L819	R820	E821	I825	Q828	M833	Y834	T835	L836	PRO	GLN	ALA	THR	PRO	GLY	VAL	PRO	GLN	GLN	SER	PRO	SER	MET																						
1	G713	I714	M715	Y616	L622	C623	T624	L625	P626	Q633	K634	L636	P635	F639	V640	P644	E645	W646	A650	G651	Q652	R653	G654	G655	N660	K661	D667	R668	G669	F670	M671	D672	P673	M674	G675	P676	G677	N678	T679	I780	S785	I786	P790	Q791	P792	I793	P794	R795	L796	G799	G800	E801	H802	T803	A704
2	S609	G524	Y526	D530	W531	H532	F533	A534	K535	L536	I537	F538	Q539	N540	A541	T542	P543	L544	L547	S548	W552	E557	L558	D556	S563	E564	L565	T566	R567	G568	N569	S572	C573	H574	P575	L576	A577	L582	D583	I584	R591	Q592	V593	L594	Y595	T596	E601	A705	L706	V707	G708	E800	H802	T803	A704
3	A411	V281	L282	I283	I284	H422	V423	Q427	K432	K433	I434	V435	Q438	E439	N446	K447	V449	K454	L455	K456	E457	L458	S466	E467	V468	R472	L479	H484	R485	P486	L487	T488	A489	K492	Q501	E505	E506	K507	L508	Y509	E510	L511	N514	P515	P516	S517	D518	E519							
4	M188	T189	S190	Q191	C195	F196	P197	D198	I199	I200	Q205	V209	F210	R214	N215	R216	T217	L218	Q219	L220	W221	P225	K226	Q237	S244	T246	V247	L248	V252	H253	S254	Y255	L256	G260	L261	I262	N263	G265	Y267	K268	R269	I270	K271	L273	H185	D186	K276								
5	ARG	LYS	GLU	ASP	GLU	SER	LEU	ALA	ASN	SER	GLY	ASP	GLU	TYR	SER	GLU	GLU	ARG	ALA	ASN	ALA	LYS	ALA	GLY	LYS	VAL	VAL	PRO	GLY	ASN	GLY	THR	ALA	GLU	ASN	THR	GLU	SER	GLY	GLY	PRO	ALA	ARG	LYS	ARG	ALA	LYS	VAL	GLU	ARG	THR	PRO			

- Chain B:  2% 16% 10% 73%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.66Å 179.02Å 234.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.00 – 3.20 98.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (98.00-3.20) 97.7 (98.00-3.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.191 , 0.227 0.194 , 0.226	Depositor DCC
R_{free} test set	802 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å ²)	77.8	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 81.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6357	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1IG2

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	1.54	52/5331 (1.0%)	1.41	50/7232 (0.7%)
2	B	1.17	1/1091 (0.1%)	1.26	4/1471 (0.3%)
All	All	1.49	53/6422 (0.8%)	1.39	54/8703 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	792	PRO	CA-C	9.15	1.64	1.52
1	A	801	GLU	C-O	-8.92	1.12	1.24
1	A	284	ILE	C-O	-8.21	1.15	1.24
1	A	639	PHE	C-O	7.74	1.33	1.23
1	A	790	PRO	N-CA	-6.91	1.38	1.47
1	A	779	PRO	N-CA	-6.79	1.38	1.47
1	A	699	LYS	C-O	-6.77	1.16	1.24
1	A	777	ALA	C-O	6.74	1.32	1.24
1	A	644	PRO	CA-C	-6.57	1.44	1.52
1	A	655	GLY	CA-C	-6.53	1.47	1.52
1	A	622	LEU	N-CA	-6.38	1.38	1.46
1	A	646	TRP	CB-CG	-6.37	1.30	1.50
1	A	764	VAL	CA-C	-6.11	1.46	1.53
1	A	799	ALA	C-O	-5.99	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	LEU	C-O	-5.98	1.17	1.24
1	A	763	TYR	N-CA	-5.98	1.38	1.45
1	A	531	TRP	C-O	-5.96	1.17	1.24
1	A	411	ALA	C-O	-5.95	1.17	1.24
1	A	200	ILE	N-CA	-5.80	1.39	1.46
1	A	808	PRO	CA-C	-5.76	1.45	1.52
1	A	828	GLN	C-O	-5.76	1.17	1.24
1	A	596	THR	CB-CG2	5.75	1.71	1.52
1	A	591	ARG	CZ-NH1	5.71	1.40	1.32
1	A	760	SER	C-O	-5.65	1.16	1.24
1	A	774	ASP	CA-C	-5.63	1.45	1.52
1	A	543	PRO	N-CA	-5.54	1.40	1.47
1	A	635	PRO	C-O	-5.53	1.16	1.23
1	A	191	GLN	C-O	-5.50	1.17	1.24
1	A	626	PRO	CA-C	-5.49	1.46	1.52
1	A	466	SER	C-O	-5.49	1.16	1.24
1	A	446	ASN	CA-C	-5.48	1.46	1.52
1	A	686	ALA	C-O	-5.48	1.17	1.24
1	A	298	GLN	C-O	-5.40	1.17	1.24
1	A	793	ILE	CA-C	5.40	1.58	1.52
1	A	814	ALA	N-CA	-5.39	1.39	1.46
1	A	538	PHE	C-O	-5.38	1.17	1.24
1	A	650	ALA	C-O	-5.36	1.17	1.24
1	A	468	VAL	C-O	-5.36	1.17	1.24
1	A	479	LEU	C-O	-5.34	1.18	1.24
2	B	368	GLU	CA-C	-5.30	1.46	1.52
1	A	772	ASP	N-CA	-5.28	1.39	1.46
1	A	548	SER	CA-C	-5.22	1.46	1.52
1	A	582	LEU	CA-C	-5.18	1.46	1.52
1	A	535	ASN	CG-ND2	-5.18	1.22	1.33
1	A	556	ASP	N-CA	5.18	1.52	1.46
1	A	768	SER	CA-CB	5.16	1.61	1.53
1	A	271	LYS	C-N	5.14	1.39	1.33
1	A	596	THR	CA-C	-5.12	1.46	1.52
1	A	815	LEU	C-O	-5.11	1.17	1.24
1	A	535	ASN	N-CA	-5.07	1.39	1.46
1	A	635	PRO	CA-C	-5.05	1.46	1.52
1	A	796	LEU	C-O	-5.03	1.18	1.24
1	A	820	ARG	CA-C	-5.01	1.46	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	802	HIS	N-CA-C	8.82	123.68	113.19
1	A	834	TYR	N-CA-C	7.63	122.02	112.87
1	A	786	ILE	N-CA-C	-7.47	99.75	107.89
1	A	768	SER	N-CA-C	-6.89	100.02	110.14
1	A	634	PRO	CA-C-N	6.71	126.74	119.90
1	A	634	PRO	C-N-CA	6.71	126.74	119.90
1	A	717	ASN	N-CA-C	6.65	121.24	113.20
1	A	777	ALA	N-CA-C	6.64	121.60	112.90
1	A	625	LEU	CA-C-N	6.48	126.50	119.89
1	A	625	LEU	C-N-CA	6.48	126.50	119.89
1	A	685	THR	N-CA-C	-6.42	104.20	111.07
1	A	770	GLY	N-CA-C	-6.39	106.43	114.16
1	A	705	ALA	N-CA-C	6.12	118.39	108.41
1	A	377	MET	CB-CG-SD	6.00	130.69	112.70
1	A	768	SER	CA-CB-OG	5.96	123.02	111.10
2	B	377	GLN	N-CA-C	5.91	118.27	108.99
1	A	809	ALA	N-CA-C	5.75	119.36	111.54
2	B	427	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	A	333	VAL	N-CA-C	5.74	116.85	108.53
1	A	273	LEU	N-CA-C	5.73	116.19	109.60
1	A	786	ILE	CA-C-N	-5.66	114.13	119.85
1	A	786	ILE	C-N-CA	-5.66	114.13	119.85
1	A	514	ASN	CA-C-N	-5.64	114.57	120.38
1	A	514	ASN	C-N-CA	-5.64	114.57	120.38
1	A	821	GLU	N-CA-C	-5.61	105.08	111.14
1	A	244	SER	N-CA-C	5.61	117.07	111.07
2	B	374	GLU	N-CA-C	5.59	117.84	108.96
1	A	624	THR	CA-CB-OG1	5.54	117.90	109.60
1	A	625	LEU	O-C-N	5.53	126.81	121.28
1	A	639	PHE	CA-C-O	5.51	126.92	120.80
1	A	281	VAL	N-CA-C	5.50	115.80	108.11
1	A	435	VAL	CB-CA-C	-5.48	104.74	112.14
2	B	426	ARG	CA-CB-CG	5.47	125.04	114.10
1	A	668	ARG	N-CA-C	5.47	117.40	108.76
1	A	472	ARG	N-CA-C	5.46	117.38	109.07
1	A	754	ASP	CA-C-N	5.44	125.53	119.87
1	A	754	ASP	C-N-CA	5.44	125.53	119.87
1	A	351	MET	N-CA-C	-5.44	101.42	110.17
1	A	458	LEU	CB-CA-C	-5.43	100.24	110.67
1	A	819	LEU	O-C-N	5.40	127.85	122.12
1	A	712	ALA	O-C-N	5.38	127.69	122.09
1	A	756	TRP	CA-C-O	5.37	125.84	119.56
1	A	817	SER	N-CA-C	-5.34	105.50	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	655	GLY	CA-C-N	-5.29	115.34	122.86
1	A	655	GLY	C-N-CA	-5.29	115.34	122.86
1	A	542	THR	N-CA-C	5.26	114.89	108.11
1	A	563	SER	N-CA-C	-5.09	103.32	110.50
1	A	271	LYS	CA-C-N	-5.07	114.44	120.11
1	A	271	LYS	C-N-CA	-5.07	114.44	120.11
1	A	515	PRO	CA-C-N	-5.06	115.56	120.98
1	A	515	PRO	C-N-CA	-5.06	115.56	120.98
1	A	172	SER	N-CA-C	5.04	116.65	109.14
1	A	281	VAL	CB-CA-C	-5.04	103.18	110.63
1	A	199	ILE	N-CA-C	5.01	115.13	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	792	PRO	Peptide
2	B	377	GLN	Peptide

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	122	0
2	B	1076	0	1090	42	0
3	A	64	0	0	2	0
All	All	6357	0	6342	154	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 12.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:ARG:CZ	2:B:431:ASP:OD1	2.03	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.55	0.89
1:A:801:GLU:HG2	1:A:809:ALA:HA	1.59	0.85
2:B:425:ARG:NH2	2:B:431:ASP:OD1	2.12	0.81
1:A:606:ASN:O	1:A:609:SER:O	2.03	0.77
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.68	0.75
1:A:771:ASN:HA	1:A:805:ARG:NH1	2.04	0.73
2:B:425:ARG:NH2	2:B:431:ASP:CG	2.46	0.73
1:A:374:LYS:O	1:A:378:VAL:HG23	1.87	0.72
1:A:526:ARG:NH1	1:A:530:ASP:OD1	2.22	0.72
1:A:384:ARG:NH2	2:B:312:LYS:O	2.23	0.71
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.20	0.71
2:B:425:ARG:NH1	2:B:431:ASP:OD1	2.26	0.69
2:B:424:TYR:CE1	2:B:427:ARG:NH1	2.58	0.69
2:B:391:ALA:HB2	2:B:409:ILE:HD11	1.72	0.69
1:A:351:MET:HA	1:A:569:ASN:HD21	1.59	0.67
1:A:538:PHE:CD1	1:A:706:LEU:HD13	2.31	0.65
2:B:377:GLN:OE1	2:B:411:ASN:HB3	1.97	0.65
2:B:374:GLU:HA	2:B:374:GLU:OE2	1.96	0.64
1:A:720:ASP:O	1:A:724:VAL:HG23	1.97	0.64
1:A:807:TYR:N	1:A:808:PRO:CD	2.61	0.63
1:A:402:ASN:O	1:A:402:ASN:OD1	2.17	0.62
1:A:374:LYS:NZ	1:A:525:ASP:OD1	2.32	0.61
2:B:391:ALA:HB2	2:B:409:ILE:CD1	2.30	0.61
1:A:540:ASN:HB3	1:A:547:LEU:HD21	1.83	0.59
2:B:403:GLN:OE1	2:B:403:GLN:HA	2.02	0.59
2:B:424:TYR:HA	2:B:427:ARG:HE	1.67	0.59
1:A:456:LYS:HA	2:B:370:TYR:CE2	2.38	0.58
1:A:448:MET:HE2	2:B:363:LEU:HD13	1.86	0.58
1:A:810:THR:HG22	3:A:901:A1IG2:CAC	2.33	0.58
1:A:537:GLU:HG2	1:A:544:LEU:CD2	2.35	0.57
1:A:467:GLU:O	1:A:468:VAL:C	2.45	0.57
1:A:533:PHE:O	1:A:537:GLU:HG3	2.05	0.57
1:A:693:LEU:HD12	1:A:694:PHE:N	2.19	0.56
1:A:332:MET:SD	1:A:661:LYS:NZ	2.79	0.56
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.87	0.55
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.42	0.55
2:B:418:LYS:O	2:B:421:PHE:HB2	2.07	0.55
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.88	0.54
1:A:538:PHE:CE1	1:A:706:LEU:HD13	2.42	0.54
1:A:401:LEU:O	1:A:402:ASN:OD1	2.25	0.54
2:B:391:ALA:CB	2:B:409:ILE:HD11	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASP:OD1	1:A:247:VAL:HG22	2.08	0.54
1:A:640:VAL:O	1:A:640:VAL:HG12	2.06	0.54
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.22	0.54
1:A:306:LEU:HD13	1:A:584:ILE:HG12	1.91	0.53
1:A:538:PHE:CE1	1:A:706:LEU:HD22	2.43	0.53
1:A:538:PHE:HE1	1:A:706:LEU:HD22	1.73	0.53
1:A:374:LYS:O	1:A:375:ASP:C	2.51	0.53
1:A:364:GLU:O	1:A:365:ALA:C	2.52	0.53
1:A:569:ASN:OD1	1:A:569:ASN:N	2.34	0.53
2:B:415:VAL:HG22	2:B:419:ASN:HD21	1.74	0.52
1:A:188:MET:HE3	1:A:210:PHE:CE2	2.43	0.52
1:A:364:GLU:OE2	1:A:524:ARG:HG2	2.10	0.52
2:B:425:ARG:NH2	2:B:431:ASP:OD2	2.41	0.52
1:A:366:ASN:OD1	1:A:367:GLY:N	2.43	0.51
1:A:772:ASP:HA	1:A:775:LEU:HD12	1.93	0.51
1:A:801:GLU:CG	1:A:809:ALA:HA	2.38	0.51
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.47	0.50
1:A:501:GLN:O	1:A:505:GLU:HB2	2.12	0.50
1:A:572:SER:O	1:A:573:CYS:C	2.55	0.50
1:A:385:LEU:O	1:A:388:ALA:HB3	2.12	0.49
1:A:510:GLU:HG3	1:A:511:LEU:HD23	1.94	0.49
1:A:606:ASN:HD22	1:A:609:SER:H	1.61	0.49
2:B:347:ARG:HG3	2:B:348:GLN:N	2.26	0.49
1:A:245:ASP:OD1	1:A:245:ASP:C	2.56	0.48
2:B:415:VAL:HG22	2:B:419:ASN:ND2	2.27	0.48
1:A:195:CYS:HB2	1:A:196:PHE:CD1	2.48	0.48
2:B:419:ASN:O	2:B:423:ASN:ND2	2.46	0.48
1:A:386:LEU:O	1:A:387:GLU:C	2.56	0.48
1:A:715:MET:HE3	1:A:723:ILE:HG12	1.95	0.48
1:A:418:LEU:HD12	2:B:324:VAL:HG21	1.95	0.48
1:A:422:HIS:CE1	2:B:315:PHE:CE1	3.02	0.47
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.96	0.47
1:A:530:ASP:OD2	1:A:685:THR:HA	2.15	0.47
1:A:693:LEU:HD12	1:A:694:PHE:H	1.79	0.47
1:A:794:PRO:HD2	1:A:828:GLN:NE2	2.30	0.47
1:A:438:GLN:HE21	1:A:508:LEU:HD13	1.80	0.47
1:A:594:ARG:HA	1:A:640:VAL:O	2.15	0.47
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.63	0.46
1:A:786:ILE:H	1:A:786:ILE:HD12	1.80	0.46
1:A:574:VAL:HB	1:A:575:PRO:CD	2.45	0.46
1:A:548:SER:O	1:A:552:TRP:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:O	1:A:272:PRO:HD3	2.16	0.46
1:A:670:PHE:C	1:A:670:PHE:CD1	2.93	0.45
1:A:771:ASN:CA	1:A:805:ARG:NH1	2.76	0.45
2:B:430:ILE:O	2:B:431:ASP:C	2.59	0.45
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.46	0.45
1:A:660:ASN:OD1	1:A:749:SER:OG	2.27	0.45
1:A:671:TRP:O	1:A:673:PRO:HD3	2.17	0.45
1:A:670:PHE:HD1	1:A:670:PHE:O	2.00	0.45
1:A:506:GLU:C	1:A:508:LEU:H	2.25	0.45
1:A:196:PHE:N	1:A:197:PRO:CD	2.80	0.45
1:A:489:ALA:O	1:A:492:LYS:HB2	2.16	0.45
1:A:288:VAL:O	1:A:289:SER:C	2.60	0.44
1:A:364:GLU:OE2	1:A:524:ARG:CG	2.64	0.44
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.99	0.44
2:B:383:TRP:O	2:B:384:THR:C	2.60	0.44
2:B:395:ILE:HG22	2:B:433:VAL:HG12	2.00	0.44
1:A:404:LYS:O	1:A:405:PRO:C	2.61	0.44
1:A:572:SER:O	1:A:574:VAL:N	2.50	0.44
1:A:804:ILE:O	1:A:808:PRO:HD3	2.18	0.44
2:B:391:ALA:O	2:B:392:VAL:C	2.59	0.44
1:A:331:ALA:HA	3:A:901:A1IG2:N5	2.33	0.44
1:A:456:LYS:HA	2:B:370:TYR:HE2	1.83	0.44
1:A:199:ILE:HD11	1:A:248:LEU:CD1	2.48	0.44
1:A:427:GLN:NE2	1:A:518:ASP:HA	2.33	0.44
1:A:654:MET:HE2	1:A:654:MET:HB3	1.78	0.44
2:B:430:ILE:HG22	2:B:434:LEU:HD12	1.99	0.43
1:A:793:ILE:HA	1:A:794:PRO:HD3	1.83	0.43
2:B:308:ARG:HH11	2:B:308:ARG:HA	1.82	0.43
1:A:205:GLN:O	1:A:209:VAL:HG23	2.19	0.43
1:A:311:ASP:OD1	1:A:311:ASP:N	2.49	0.43
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.59	0.43
1:A:700:ALA:HB1	1:A:701:PRO:HD2	2.01	0.43
1:A:266:ILE:CD1	1:A:577:ALA:HB1	2.49	0.42
1:A:487:LEU:HD21	2:B:370:TYR:O	2.19	0.42
1:A:633:GLN:HA	1:A:634:PRO:HA	1.74	0.42
2:B:414:VAL:O	2:B:414:VAL:HG12	2.19	0.42
2:B:314:MET:HB2	2:B:314:MET:HE2	1.84	0.42
1:A:771:ASN:HA	1:A:805:ARG:HH11	1.80	0.42
1:A:506:GLU:C	1:A:508:LEU:N	2.78	0.42
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.55	0.42
1:A:181:SER:OG	1:A:218:LEU:HD22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:ILE:O	2:B:409:ILE:HG22	2.18	0.42
1:A:353:LEU:HB3	1:A:565:LEU:HD22	2.02	0.42
1:A:707:VAL:HG12	1:A:712:ALA:HA	2.02	0.42
1:A:214:ARG:HD2	1:A:215:ASN:OD1	2.19	0.41
1:A:260:GLY:O	1:A:264:PHE:CD2	2.73	0.41
2:B:401:ASP:O	2:B:402:PHE:C	2.63	0.41
1:A:563:SER:O	1:A:565:LEU:HD12	2.20	0.41
1:A:806:ASN:C	1:A:807:TYR:CD1	2.99	0.41
1:A:183:LEU:HD23	1:A:189:THR:HG21	2.01	0.41
1:A:216:ARG:O	1:A:220:LEU:HD12	2.21	0.41
1:A:252:VAL:O	1:A:253:HIS:C	2.64	0.41
1:A:217:THR:HA	1:A:220:LEU:HD12	2.03	0.41
1:A:221:TRP:CZ3	1:A:225:PRO:HA	2.55	0.41
1:A:538:PHE:CE1	1:A:706:LEU:CD1	3.03	0.41
1:A:255:TYR:CE2	1:A:256:LEU:HD23	2.56	0.41
1:A:507:LYS:O	1:A:507:LYS:HG2	2.21	0.41
1:A:601:GLU:HA	1:A:616:TYR:O	2.20	0.41
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.56	0.41
1:A:485:ARG:HG3	2:B:407:ASP:HB2	2.03	0.41
1:A:538:PHE:CE1	1:A:706:LEU:CD2	3.04	0.41
2:B:389:LEU:O	2:B:390:LEU:C	2.63	0.41
1:A:537:GLU:HG2	1:A:544:LEU:HD23	2.00	0.40
1:A:722:VAL:O	1:A:726:ARG:HG3	2.21	0.40
2:B:383:TRP:CE3	2:B:412:LYS:HE2	2.55	0.40
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.90	0.40
1:A:468:VAL:O	1:A:472:ARG:NH1	2.54	0.40
1:A:245:ASP:OD1	1:A:247:VAL:CG2	2.68	0.40
1:A:340:ASN:O	1:A:343:ALA:HB3	2.20	0.40
1:A:536:LEU:HB3	1:A:544:LEU:HD21	2.04	0.40
2:B:403:GLN:OE1	2:B:414:VAL:HG22	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	664/852 (78%)	602 (91%)	57 (9%)	5 (1%)	16	50
2	B	131/485 (27%)	117 (89%)	13 (10%)	1 (1%)	16	50
All	All	795/1337 (60%)	719 (90%)	70 (9%)	6 (1%)	16	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	793	ILE
1	A	801	GLU
1	A	507	LYS
1	A	271	LYS
2	B	439	ALA
1	A	364	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	566/699 (81%)	526 (93%)	40 (7%)	13	44
2	B	117/397 (30%)	101 (86%)	16 (14%)	3	18
All	All	683/1096 (62%)	627 (92%)	56 (8%)	10	39

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LEU
1	A	205	GLN
1	A	226	LYS
1	A	237	GLN
1	A	268	LYS
1	A	276	LYS
1	A	299	SER

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Mol	Chain	Res	Type
1	A	372	LYS
1	A	378	VAL
1	A	380	GLN
1	A	422	HIS
1	A	423	VAL
1	A	432	LYS
1	A	433	LYS
1	A	434	ILE
1	A	439	GLU
1	A	447	LYS
1	A	449	VAL
1	A	454	LYS
1	A	485	ARG
1	A	517	SER
1	A	563	SER
1	A	567	VAL
1	A	569	ASN
1	A	591	ARG
1	A	624	THR
1	A	645	GLU
1	A	652	GLN
1	A	667	ASP
1	A	675	VAL
1	A	714	ILE
1	A	718	ILE
1	A	737	SER
1	A	780	ILE
1	A	785	SER
1	A	786	ILE
1	A	791	GLN
1	A	793	ILE
1	A	815	LEU
1	A	825	ILE
2	B	308	ARG
2	B	316	LEU
2	B	317	SER
2	B	334	VAL
2	B	343	VAL
2	B	345	VAL
2	B	346	LYS
2	B	347	ARG
2	B	355	THR

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Mol	Chain	Res	Type
2	B	374	GLU
2	B	376	ILE
2	B	378	LYS
2	B	379	CYS
2	B	385	THR
2	B	422	VAL
2	B	426	ARG

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	259	HIS
1	A	380	GLN
1	A	422	HIS
1	A	438	GLN
1	A	551	HIS
1	A	554	GLN
1	A	632	GLN
1	A	742	GLN
1	A	828	GLN
2	B	350	GLN
2	B	411	ASN
2	B	419	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	A1IG2	A	901	-	68,71,71	2.15	23 (33%)	93,111,111	2.02	21 (22%)

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	A1IG2	A	901	-	-	3/38/106/106	0/7/8/8

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	A1IG2	CAD-CAB	5.48	1.47	1.39
3	A	901	A1IG2	CAC-CAE	4.99	1.46	1.37
3	A	901	A1IG2	CAF-CAE	4.93	1.46	1.37
3	A	901	A1IG2	CAC-CAA	4.93	1.46	1.38
3	A	901	A1IG2	P-O3P	4.63	1.64	1.59
3	A	901	A1IG2	CAF-CAD	4.01	1.45	1.38
3	A	901	A1IG2	PA-O3P	3.84	1.63	1.59
3	A	901	A1IG2	C5A-C4A	3.71	1.45	1.39
3	A	901	A1IG2	CAA-CAB	3.59	1.44	1.39
3	A	901	A1IG2	C5X-C9A	3.47	1.47	1.41
3	A	901	A1IG2	C1'-C2'	3.06	1.56	1.52
3	A	901	A1IG2	C5A-N7A	-2.94	1.33	1.39
3	A	901	A1IG2	C5'-C4'	2.86	1.55	1.51
3	A	901	A1IG2	C10-N1	2.73	1.39	1.31
3	A	901	A1IG2	C6-C7	-2.63	1.36	1.39
3	A	901	A1IG2	C8A-N9A	-2.44	1.33	1.37
3	A	901	A1IG2	CCA-CBZ	-2.35	1.50	1.55
3	A	901	A1IG2	O4-C4	2.27	1.26	1.22
3	A	901	A1IG2	O2-C2	2.27	1.28	1.24
3	A	901	A1IG2	C5X-N5	-2.26	1.37	1.41
3	A	901	A1IG2	C8-C7	2.23	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	A1IG2	C4A-N3A	2.15	1.38	1.34
3	A	901	A1IG2	C5A-C6A	2.10	1.46	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	A1IG2	N3A-C4A-N9A	6.26	137.81	127.17
3	A	901	A1IG2	C5X-N5-CCB	-6.22	109.66	123.92
3	A	901	A1IG2	C5A-C4A-N3A	-5.68	118.89	126.72
3	A	901	A1IG2	N1A-C2A-N3A	-5.34	120.50	128.58
3	A	901	A1IG2	O3P-P-O1P	-4.55	97.02	110.70
3	A	901	A1IG2	C2A-N3A-C4A	4.41	122.60	111.83
3	A	901	A1IG2	C4A-N9A-C8A	3.95	109.89	105.74
3	A	901	A1IG2	C5A-C6A-N6A	-3.78	113.92	123.29
3	A	901	A1IG2	N6A-C6A-N1A	3.63	126.47	118.38
3	A	901	A1IG2	O5'-P-O1P	3.23	121.74	108.94
3	A	901	A1IG2	CCA-CBZ-CAB	-3.20	110.38	116.60
3	A	901	A1IG2	C4X-N5-CCB	2.94	112.45	109.50
3	A	901	A1IG2	O5'-C5'-C4'	2.88	117.06	109.36
3	A	901	A1IG2	O4'-C4'-C3'	2.46	115.01	109.25
3	A	901	A1IG2	O2A-PA-O1A	2.42	123.68	112.44
3	A	901	A1IG2	C9-C9A-C5X	-2.37	116.42	120.06
3	A	901	A1IG2	C5A-C4A-N9A	-2.33	103.28	105.81
3	A	901	A1IG2	C5'-C4'-C3'	-2.29	107.89	112.22
3	A	901	A1IG2	C9A-C5X-N5	2.09	124.84	120.11
3	A	901	A1IG2	C8M-C8-C7	-2.02	116.63	120.76
3	A	901	A1IG2	CAA-CAB-CBZ	-2.00	117.07	121.07

There are no chirality outliers.

All (3) torsion outliers are listed below:

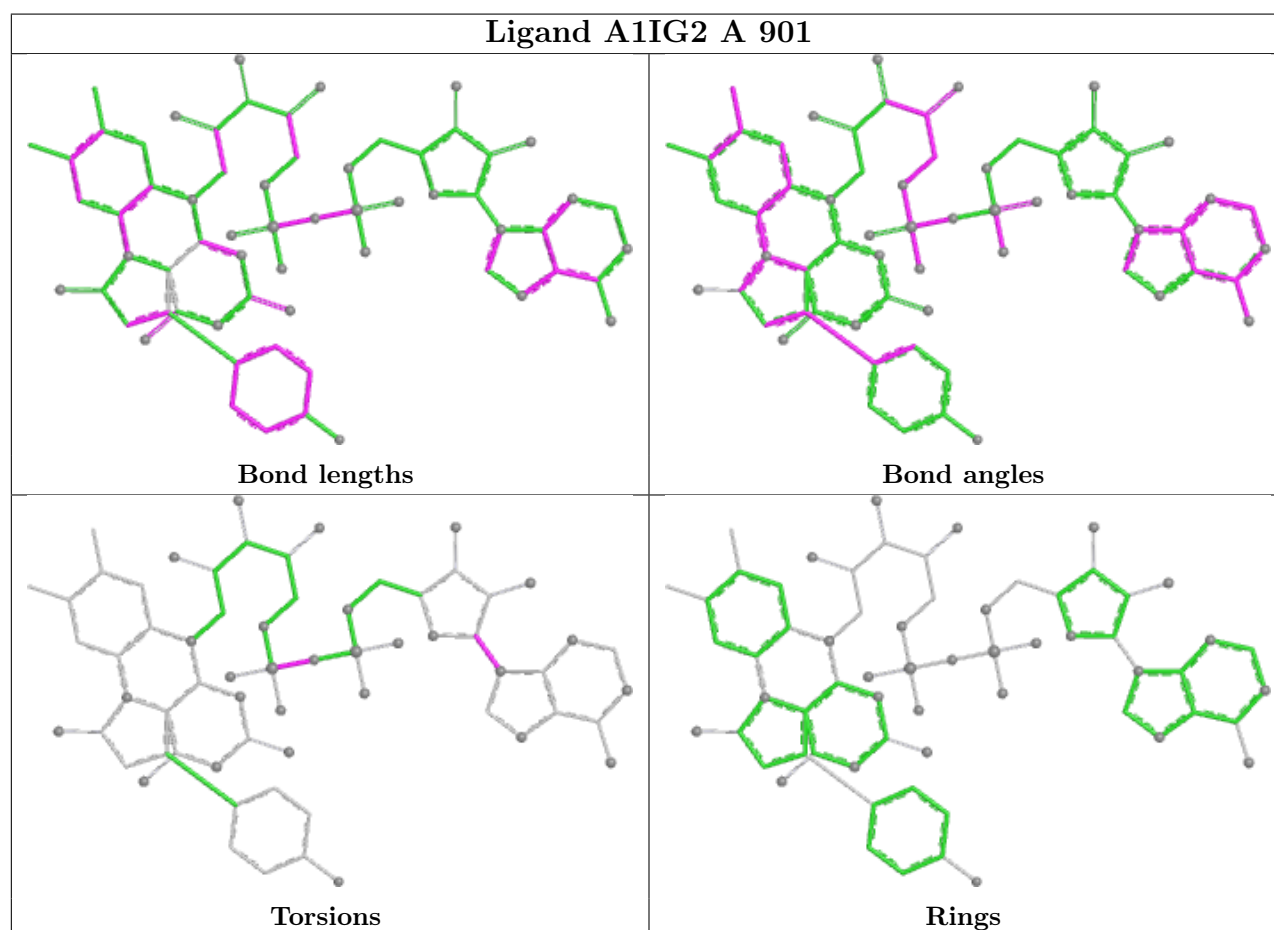
Mol	Chain	Res	Type	Atoms
3	A	901	A1IG2	C2B-C1B-N9A-C8A
3	A	901	A1IG2	PA-O3P-P-O5'
3	A	901	A1IG2	O4B-C1B-N9A-C8A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	A1IG2	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	666/852 (78%)	-0.29	6 (0%) 81 64	45, 75, 112, 139	0
2	B	133/485 (27%)	0.18	8 (6%) 27 17	76, 106, 134, 141	0
All	All	799/1337 (59%)	-0.21	14 (1%) 67 48	45, 81, 120, 141	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	4.1
1	A	836	LEU	3.4
2	B	337	GLN	3.2
2	B	426	ARG	2.8
2	B	376	ILE	2.8
1	A	833	MET	2.6
2	B	340	MET	2.5
1	A	272	PRO	2.4
2	B	374	GLU	2.3
2	B	440	GLU	2.3
2	B	308	ARG	2.3
1	A	377	MET	2.3
1	A	380	GLN	2.1
2	B	427	ARG	2.1

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](#)

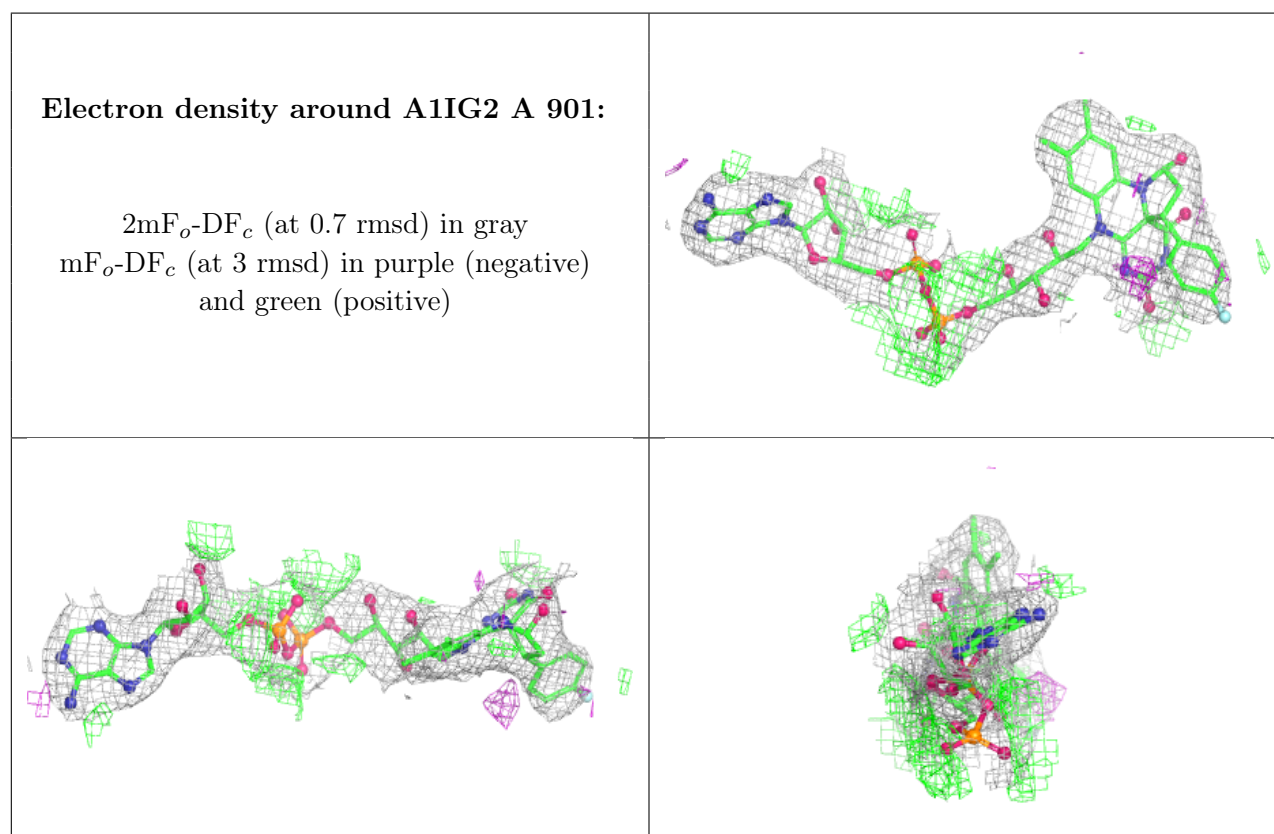
There are no oligosaccharides in this entry.

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
3	A1IG2	A	901	64/64	0.97	0.08	41,58,70,93	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.