



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:05 PM UTC

PDB ID : 1H8S / pdb_00001h8s
Title : Three-dimensional structure of anti-ampicillin single chain Fv fragment complexed with the hapten.
Authors : Burmester, J.; Spinelli, S.; Pugliese, L.; Krebber, A.; Honegger, A.; Jung, S.; Schimmele, B.; Cambillau, C.; Pluckthun, A.
Deposited on : 2001-02-15
Resolution : 2.40 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

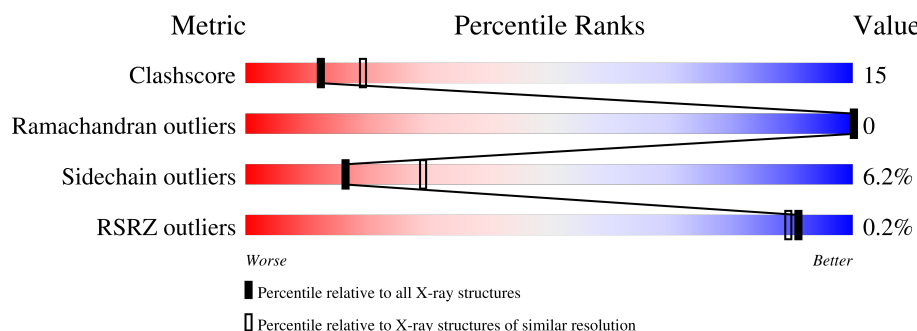
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
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	252	
1	B	252	

2 Entry composition [i](#)

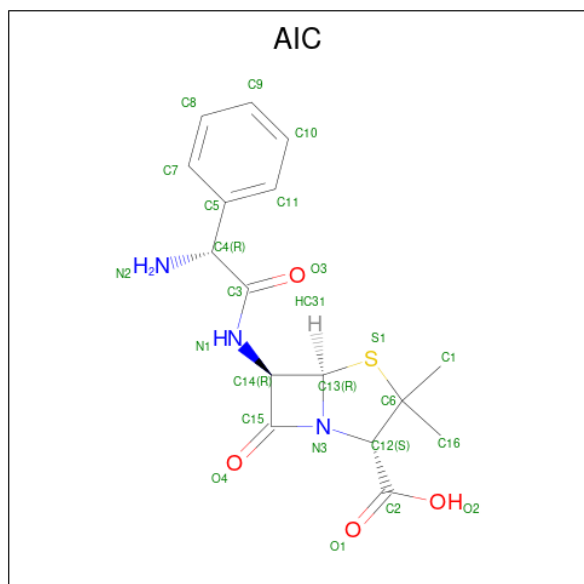
There are 4 unique types of molecules in this entry. The entry contains 3731 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MUTANT AL2 6E7P9G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	1	2
			1695	1075	281	333	6			
1	B	220	Total	C	N	O	S	0	0	2
			1705	1081	285	333	6			

- Molecule 2 is (2S,5R,6R)-6-[(2R)-2-AMINO-2-PHENYLETHANOYL]AMINO}-3,3-DIMETHYL-7-OXO-4-THIA-1-AZABICYCLO[3.2.0]HEPTANE-2-CARBOXYLIC ACID (CCD ID: AIC) (formula: C₁₆H₁₉N₃O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	16	3	4	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

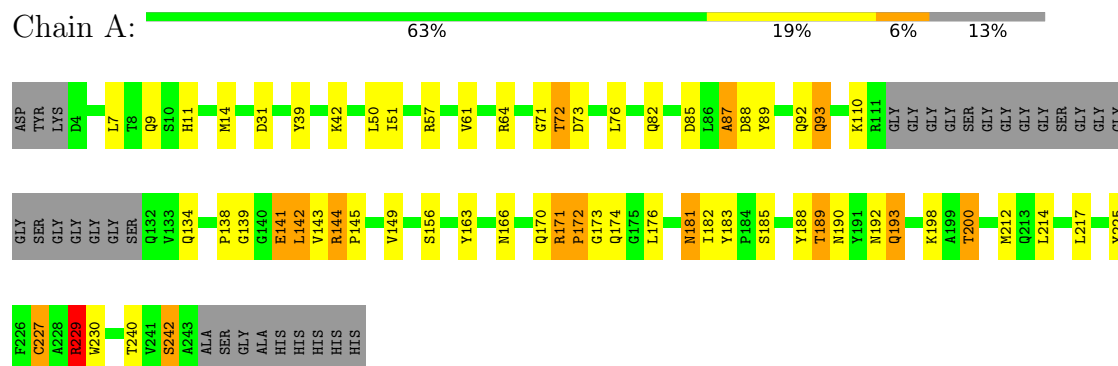
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total	O	0	0
			159	159		
4	B	138	Total	O	0	0
			138	138		

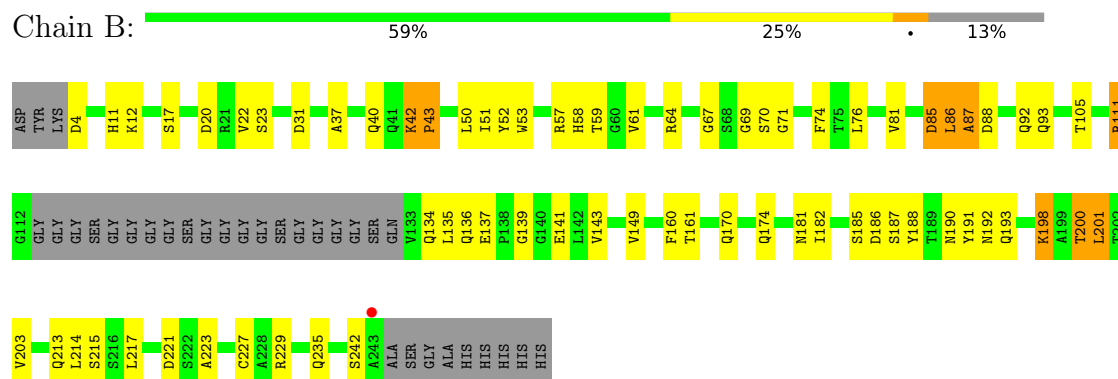
3 Residue-property plots

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: MUTANT AL2 6E7P9G



• Molecule 1: MUTANT AL2 6E7P9G



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.93Å 89.27Å 94.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.94 – 2.40 12.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (12.94-2.40) 96.4 (12.94-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.273 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3731	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AIC, SO4

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	0.75	6/1727 (0.3%)	1.06	7/2349 (0.3%)
1	B	0.79	8/1748 (0.5%)	1.06	11/2376 (0.5%)
All	All	0.77	14/3475 (0.4%)	1.06	18/4725 (0.4%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	42	LYS	C-N	-10.44	1.09	1.33
1	B	85	ASP	C-N	-7.50	1.22	1.33
1	A	171	ARG	C-N	-7.26	1.16	1.33
1	B	43	PRO	N-CD	-7.04	1.37	1.47
1	B	86	LEU	C-N	-6.67	1.23	1.33
1	A	173	GLY	N-CA	-6.56	1.35	1.45
1	A	172	PRO	N-CD	-6.50	1.38	1.47
1	B	87	ALA	N-CA	-6.31	1.38	1.46
1	B	111	ARG	C-N	-5.76	1.25	1.33
1	A	242	SER	C-N	-5.63	1.25	1.33
1	A	172	PRO	C-N	-5.42	1.25	1.33
1	A	110	LYS	C-N	-5.31	1.25	1.33
1	B	86	LEU	CA-C	-5.22	1.46	1.52
1	B	242	SER	C-N	-5.21	1.26	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	LYS	CA-C-N	7.08	128.68	119.84
1	B	42	LYS	C-N-CA	7.08	128.68	119.84
1	B	227	CYS	N-CA-C	-7.07	97.88	109.40
1	A	192	ASN	N-CA-C	-7.03	98.49	109.25
1	A	87	ALA	O-C-N	7.02	130.34	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	ARG	N-CA-C	-6.76	100.51	110.52
1	A	171	ARG	CA-C-N	6.72	128.24	119.84
1	A	171	ARG	C-N-CA	6.72	128.24	119.84
1	B	192	ASN	N-CA-C	-6.66	99.17	109.76
1	A	227	CYS	N-CA-C	-6.37	99.53	109.72
1	A	139	GLY	N-CA-C	-5.94	102.87	112.31
1	B	188	TYR	N-CA-C	-5.93	101.27	110.10
1	B	174	GLN	N-CA-C	5.79	117.37	110.19
1	B	160	PHE	N-CA-C	5.61	118.12	111.33
1	B	139	GLY	N-CA-C	-5.34	103.82	112.31
1	B	134	GLN	N-CA-C	5.23	117.34	109.23
1	A	229	ARG	N-CA-C	-5.12	101.80	109.95
1	B	69	GLY	N-CA-C	5.08	117.22	112.04

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	1695	0	1614	58	0
1	B	1705	0	1638	44	0
2	A	24	0	18	6	0
3	A	10	0	0	1	0
4	A	159	0	0	9	0
4	B	138	0	0	4	0
All	All	3731	0	3270	103	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 15.

All (103) 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:A:1000:AIC:O2	4:A:2157:HOH:O	1.87	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLN:H	1:A:193:GLN:NE2	1.68	0.90
1:A:230[H]:TRP:CE3	2:A:1000:AIC:N2	2.49	0.80
1:A:144:ARG:HG3	1:A:145:PRO:HD2	1.66	0.78
1:A:230[H]:TRP:HE3	2:A:1000:AIC:HN22	1.31	0.77
1:A:181:ASN:HD21	1:A:190:ASN:HD22	1.36	0.73
1:A:181:ASN:ND2	1:A:190:ASN:HB2	2.04	0.73
1:A:193:GLN:H	1:A:193:GLN:CD	1.95	0.73
1:B:17:SER:HB2	1:B:20:ASP:OD2	1.90	0.71
1:B:31:ASP:OD1	1:B:71:GLY:HA2	1.93	0.69
1:B:235:GLN:HG2	4:B:2039:HOH:O	1.93	0.69
2:A:1000:AIC:S1	4:A:2158:HOH:O	2.52	0.68
1:A:181:ASN:HD21	1:A:190:ASN:HB2	1.62	0.63
1:A:182:ILE:HG13	1:A:189:THR:HG22	1.80	0.63
1:B:40:GLN:HB2	1:B:50:LEU:HD11	1.82	0.61
3:A:1002:SO4:O1	1:B:111:ARG:HD3	2.00	0.60
1:A:64:ARG:NH1	1:A:85:ASP:OD2	2.35	0.60
1:B:198:LYS:HE2	1:B:215:SER:O	2.03	0.59
1:B:200:THR:HG22	4:B:2115:HOH:O	2.01	0.59
1:B:58:HIS:CG	1:B:59:THR:H	2.21	0.58
1:A:11:HIS:HD2	1:A:14:MET:HE2	1.68	0.58
1:B:143:VAL:HG21	1:B:217:LEU:HD13	1.86	0.58
1:B:170:GLN:O	1:B:223:ALA:HB1	2.02	0.58
1:B:12:LYS:HG3	4:B:2071:HOH:O	2.03	0.58
1:A:142:LEU:HD21	1:A:242:SER:HB2	1.87	0.57
1:A:230[H]:TRP:CZ3	2:A:1000:AIC:N2	2.70	0.56
1:A:143:VAL:HG21	1:A:217:LEU:HD13	1.87	0.55
1:A:7:LEU:HD11	1:A:93:GLN:CB	2.37	0.55
1:B:11:HIS:O	1:B:105:THR:HG23	2.07	0.55
1:A:57:ARG:HD3	1:A:61:VAL:O	2.06	0.55
1:B:200:THR:CG2	4:B:2115:HOH:O	2.55	0.55
1:A:7:LEU:HD11	1:A:93:GLN:HB2	1.88	0.55
1:A:50:LEU:O	1:A:51:ILE:HD13	2.06	0.55
1:B:58:HIS:CG	1:B:59:THR:N	2.74	0.55
1:B:182:ILE:HD13	1:B:203:VAL:HG13	1.89	0.55
1:A:189:THR:HG21	4:A:2136:HOH:O	2.06	0.54
1:A:50:LEU:HA	1:A:61:VAL:HG21	1.89	0.54
1:A:170:GLN:HB2	1:A:176:LEU:CD2	2.38	0.54
1:A:57:ARG:HH21	1:A:57:ARG:HB3	1.75	0.52
1:B:149:VAL:HG12	1:B:214:LEU:HB2	1.90	0.52
1:B:191:TYR:HE1	1:B:201:LEU:HD13	1.74	0.51
1:A:166:ASN:O	1:A:227:CYS:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASP:HA	1:A:71:GLY:O	2.12	0.50
1:B:20:ASP:O	1:B:81:VAL:HG23	2.11	0.50
1:A:183:TYR:CE2	1:A:185:SER:HB3	2.47	0.50
1:A:72:THR:HG22	1:A:73:ASP:OD2	2.11	0.50
1:A:170:GLN:HB2	1:A:176:LEU:HD23	1.93	0.50
1:A:230[H]:TRP:HE3	2:A:1000:AIC:N2	1.98	0.50
1:B:42:LYS:HB3	1:B:43:PRO:HD2	1.94	0.50
1:B:191:TYR:CE1	1:B:201:LEU:HD13	2.47	0.50
1:A:144:ARG:HG3	1:A:145:PRO:CD	2.40	0.50
1:B:186:ASP:O	1:B:187:SER:HB2	2.12	0.50
1:A:72:THR:CG2	1:A:73:ASP:OD2	2.60	0.49
1:A:193:GLN:H	1:A:193:GLN:HE21	1.53	0.49
1:B:22:VAL:HG12	1:B:23:SER:N	2.27	0.49
1:B:42:LYS:CB	1:B:43:PRO:HD2	2.40	0.49
1:A:57:ARG:CB	1:A:57:ARG:NH2	2.76	0.49
1:B:64:ARG:NH1	1:B:85:ASP:OD1	2.45	0.49
1:A:156:SER:HB3	4:A:2092:HOH:O	2.12	0.49
1:A:163:TYR:CD2	1:A:229:ARG:HD3	2.47	0.49
1:A:174:GLN:HG2	4:A:2106:HOH:O	2.13	0.48
1:B:57:ARG:HH11	1:B:57:ARG:HB2	1.78	0.48
1:A:39:TYR:HE2	1:A:92:GLN:HE21	1.59	0.48
1:A:57:ARG:HH21	1:A:57:ARG:CB	2.27	0.48
1:A:143:VAL:HG21	1:A:217:LEU:CD1	2.43	0.48
1:A:57:ARG:NH2	1:A:57:ARG:HB2	2.30	0.47
1:B:53:TRP:HA	1:B:53:TRP:CE3	2.50	0.47
1:A:182:ILE:HA	1:A:188:TYR:O	2.15	0.47
1:B:31:ASP:HA	1:B:71:GLY:O	2.14	0.46
1:B:51:ILE:HD13	1:B:67:GLY:N	2.30	0.46
1:A:141:GLU:N	1:A:141:GLU:CD	2.74	0.46
1:B:181:ASN:OD1	1:B:190:ASN:HB2	2.16	0.46
1:B:217:LEU:HA	1:B:221:ASP:OD1	2.16	0.46
1:A:166:ASN:OD1	1:A:181:ASN:HB3	2.16	0.46
1:B:50:LEU:HA	1:B:61:VAL:HG21	1.98	0.46
1:A:134:GLN:HB2	4:A:2081:HOH:O	2.16	0.45
1:B:57:ARG:HB2	1:B:57:ARG:NH1	2.31	0.45
1:A:42:LYS:HD3	1:A:87:ALA:HB2	1.97	0.45
1:A:181:ASN:C	1:A:181:ASN:HD22	2.24	0.45
1:B:37:ALA:HB3	1:B:92:GLN:HE21	1.81	0.45
1:A:9:GLN:HB3	1:B:111:ARG:NH2	2.33	0.44
1:B:135:LEU:O	1:B:137:GLU:HG3	2.16	0.44
1:A:171:ARG:HD3	4:A:2104:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:HG23	1:B:213:GLN:HB3	2.00	0.44
1:A:142:LEU:HD23	1:A:240:THR:CG2	2.47	0.43
1:A:39:TYR:O	1:A:89:TYR:HA	2.18	0.43
1:A:82:GLN:O	1:A:85:ASP:HB2	2.19	0.42
1:A:200:THR:HG22	4:A:2143:HOH:O	2.19	0.42
1:A:212:MET:HE1	1:A:225:TYR:CD2	2.55	0.42
1:A:142:LEU:C	1:A:142:LEU:HD13	2.44	0.42
1:B:141:GLU:OE2	1:B:149:VAL:CG2	2.68	0.42
1:A:93:GLN:OE1	1:A:93:GLN:C	2.63	0.42
1:A:198:LYS:O	1:A:214:LEU:HA	2.20	0.42
1:B:22:VAL:CG1	1:B:23:SER:N	2.83	0.42
1:B:86:LEU:O	1:B:87:ALA:HB2	2.18	0.42
1:B:143:VAL:HG21	1:B:217:LEU:CD1	2.50	0.42
1:A:171:ARG:CB	1:A:172:PRO:HD2	2.50	0.41
1:A:200:THR:CG2	4:A:2143:HOH:O	2.68	0.41
1:B:135:LEU:O	1:B:136:GLN:C	2.64	0.41
1:B:161:THR:O	1:B:185:SER:HB2	2.20	0.41
1:B:70:SER:HA	1:B:74:PHE:CE1	2.56	0.41
1:B:51:ILE:HD13	1:B:67:GLY:H	1.86	0.40
1:A:181:ASN:HD21	1:A:190:ASN:ND2	2.11	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	216/252 (86%)	203 (94%)	13 (6%)	0	100	100
1	B	216/252 (86%)	204 (94%)	12 (6%)	0	100	100
All	All	432/504 (86%)	407 (94%)	25 (6%)	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	184/201 (92%)	170 (92%)	14 (8%)	12	21
1	B	187/201 (93%)	178 (95%)	9 (5%)	23	40
All	All	371/402 (92%)	348 (94%)	23 (6%)	16	29

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	76	LEU
1	A	88	ASP
1	A	93	GLN
1	A	138	PRO
1	A	141	GLU
1	A	142	LEU
1	A	144	ARG
1	A	149	VAL
1	A	181	ASN
1	A	189	THR
1	A	193	GLN
1	A	200	THR
1	A	229	ARG
1	B	4	ASP
1	B	52	TYR
1	B	76	LEU
1	B	88	ASP
1	B	93	GLN
1	B	193	GLN
1	B	198	LYS
1	B	200	THR
1	B	201	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	40	GLN
1	A	41	GLN
1	A	80	ASN
1	A	82	GLN
1	A	92	GLN
1	A	170	GLN
1	A	174	GLN
1	A	181	ASN
1	A	193	GLN
1	B	30	GLN
1	B	41	GLN
1	B	45	GLN
1	B	58	HIS
1	B	82	GLN
1	B	92	GLN
1	B	134	GLN
1	B	170	GLN
1	B	193	GLN
1	B	235	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](#)

3 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
3	SO4	A	1001	-	4,4,4	1.91	2 (50%)	6,6,6	0.85	0
2	AIC	A	1000	-	24,26,26	2.71	10 (41%)	36,40,40	1.89	9 (25%)
3	SO4	A	1002	-	4,4,4	1.79	2 (50%)	6,6,6	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AIC	A	1000	-	-	0/16/47/47	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	AIC	C5-C4	-5.88	1.46	1.52
2	A	1000	AIC	C14-C15	-5.07	1.43	1.54
2	A	1000	AIC	C6-S1	-4.55	1.76	1.85
2	A	1000	AIC	C3-N1	4.35	1.43	1.34
2	A	1000	AIC	C12-N3	4.25	1.53	1.46
2	A	1000	AIC	C12-C2	-4.15	1.48	1.53
3	A	1001	SO4	O1-S	3.11	1.63	1.44
3	A	1002	SO4	O1-S	2.91	1.62	1.44
2	A	1000	AIC	C13-C14	-2.81	1.51	1.56
2	A	1000	AIC	C7-C5	2.18	1.42	1.39
3	A	1001	SO4	O3-S	-2.15	1.30	1.48
2	A	1000	AIC	C14-N1	-2.12	1.41	1.45
2	A	1000	AIC	C15-N3	2.11	1.42	1.37
3	A	1002	SO4	O3-S	-2.03	1.31	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	AIC	C4-C3-N1	3.94	119.50	114.68
2	A	1000	AIC	C13-C14-N1	-3.86	110.49	118.49
2	A	1000	AIC	C13-N3-C12	-3.74	112.90	117.30
2	A	1000	AIC	C13-N3-C15	-3.59	89.51	93.92
2	A	1000	AIC	C14-C13-S1	3.50	124.72	119.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	AIC	C6-S1-C13	2.86	100.92	93.42
2	A	1000	AIC	C14-N1-C3	-2.83	114.90	121.90
2	A	1000	AIC	O2-C2-C12	2.76	120.40	112.47
2	A	1000	AIC	C6-C12-N3	2.05	109.40	106.43

There are no chirality outliers.

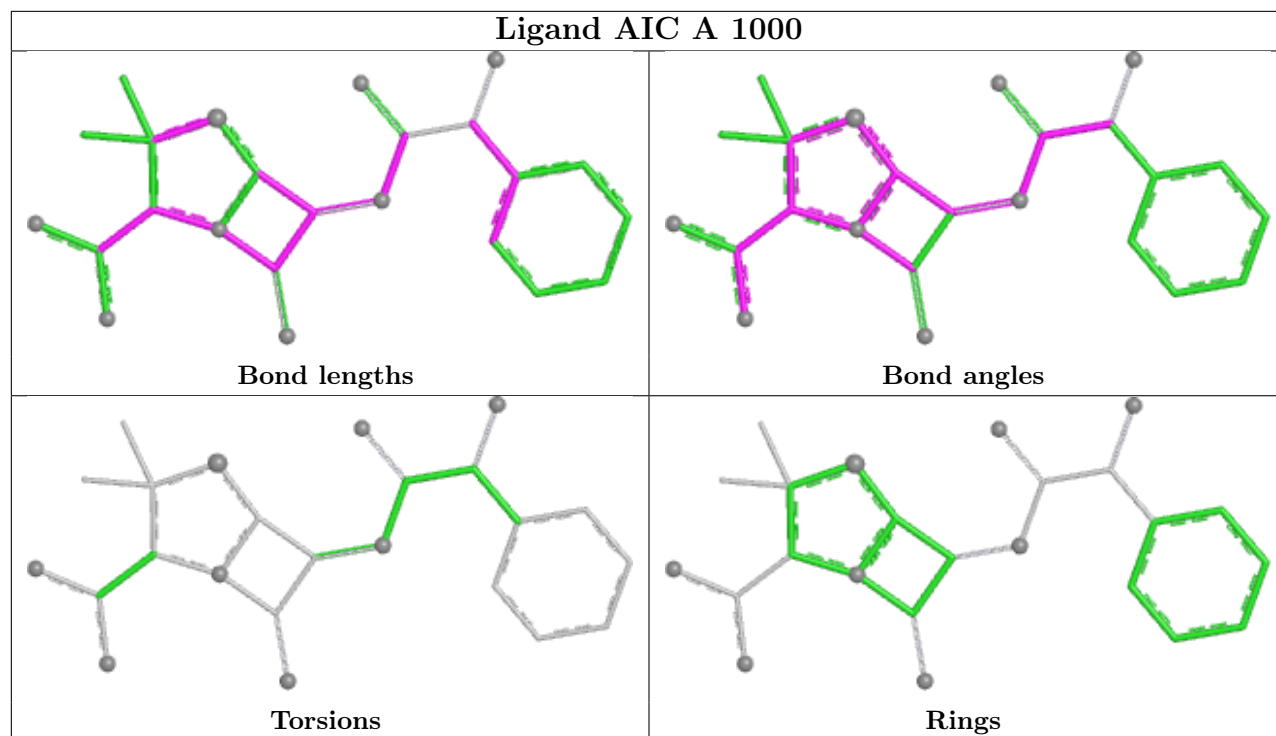
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	AIC	6	0
3	A	1002	SO4	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	171:ARG	C	172:PRO	N	1.16
1	B	42:LYS	C	43:PRO	N	1.09

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	220/252 (87%)	-0.53	0	100 100	6, 18, 34, 50	1 (0%)
1	B	220/252 (87%)	-0.40	1 (0%)	87 85	9, 23, 42, 50	0
All	All	440/504 (87%)	-0.47	1 (0%)	91 89	6, 21, 40, 50	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ALA	2.4

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](#)

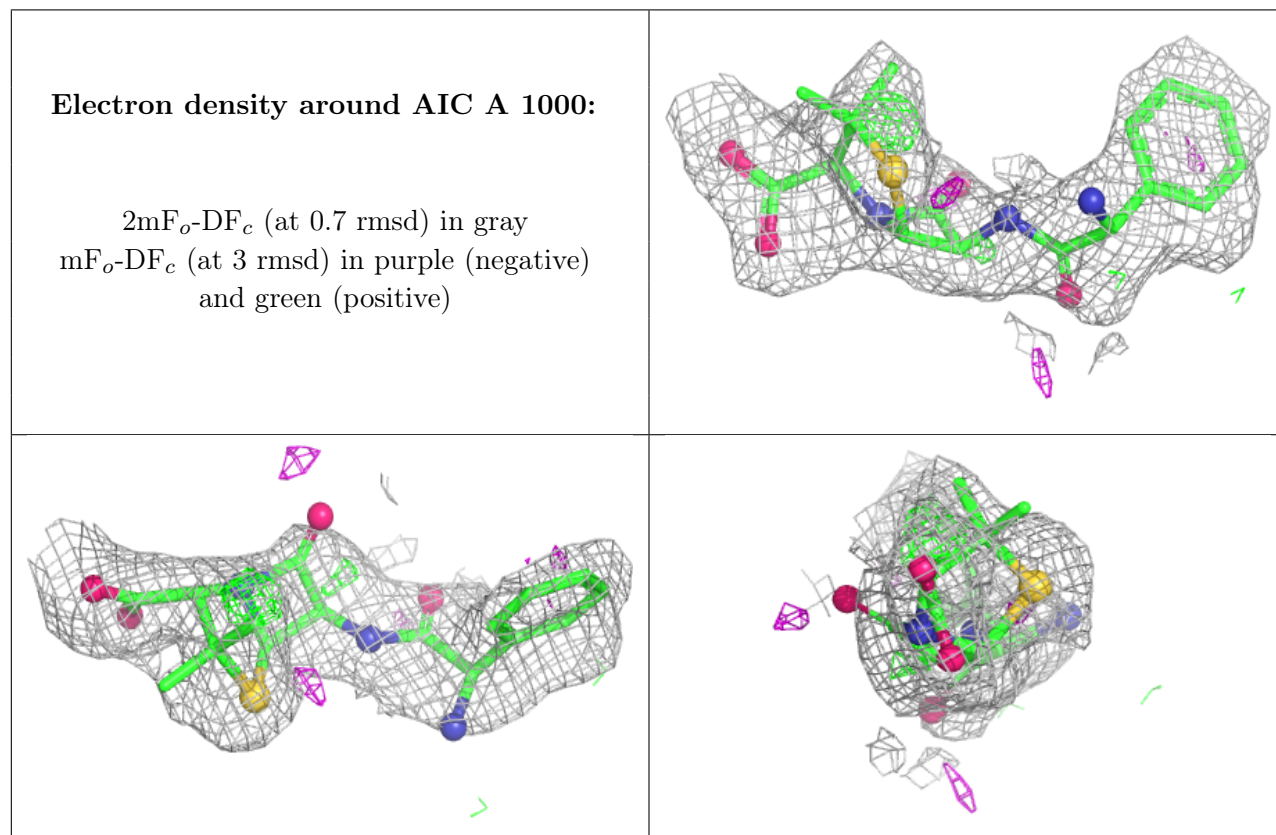
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
2	AIC	A	1000	24/24	0.82	0.15	37,55,61,64	0
3	SO4	A	1002	5/5	0.95	0.07	26,34,37,42	0
3	SO4	A	1001	5/5	0.99	0.06	21,25,29,30	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.