Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:46 am BST

PDB ID	:	1DBK
Title	:	MOLECULAR BASIS OF CROSS-REACTIVITY AND THE LIMITS OF ANTIBODY-ANTIGEN COMPLEMENTARITY
Authors	:	Arevalo, J.H.; Wilson, I.A.
Deposited on	:	1993-08-24
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

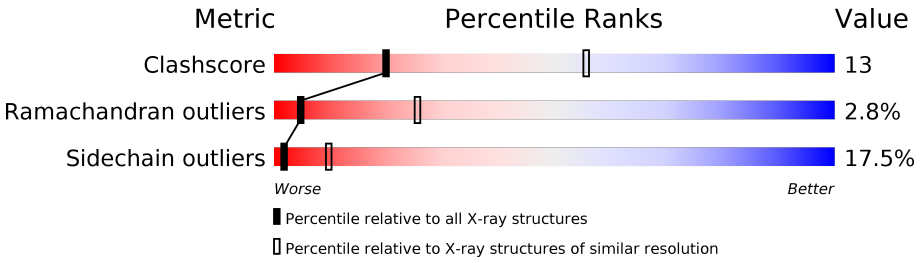
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	216	55% 37% 7% .
2	H	219	55% 33% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3377 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 IGG1-KAPPA DB3 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1679	1051	286	335	7			

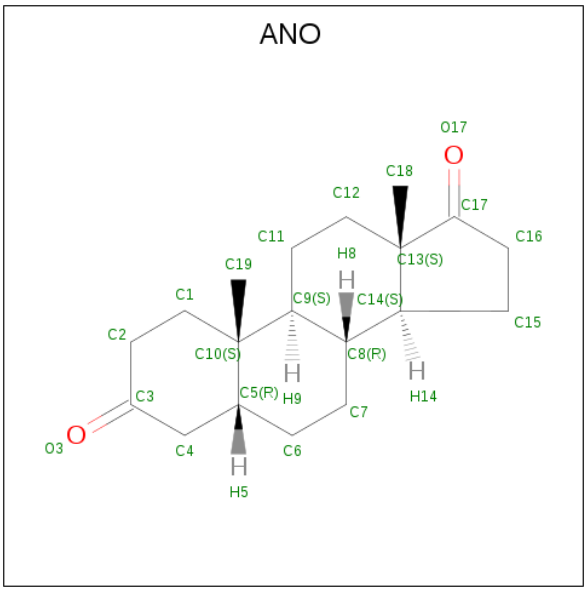
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	VAL	ILE	CONFLICT	GB 1589925
L	7	ILE	SER	CONFLICT	GB 1589925
L	14	ASN	SER	CONFLICT	GB 1589925
L	27B	LEU	VAL	CONFLICT	GB 1589925
L	27C	ILE	VAL	CONFLICT	GB 1589925
L	34	HIS	GLU	CONFLICT	GB 1589925
L	36	TYR	PHE	CONFLICT	GB 1589925
L	48	MET	ILE	CONFLICT	GB 1589925
L	56	TYR	SER	CONFLICT	GB 1589925
L	85	ILE	VAL	CONFLICT	GB 1589925
L	87	PHE	TYR	CONFLICT	GB 1589925
L	89	SER	PHE	CONFLICT	GB 1589925
L	91	SER	ALA	CONFLICT	GB 1589925
L	96	PRO	TRP	CONFLICT	GB 1589925

- Molecule 2 is a protein called IGG1-KAPPA DB3 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1675	1071	270	328	6			

- Molecule 3 is 5-BETA-ANDROSTANE-3,17-DIONE (three-letter code: ANO) (formula: $C_{19}H_{28}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 21 19 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O 1 1	0	0
4	H	1	Total O 1 1	0	0

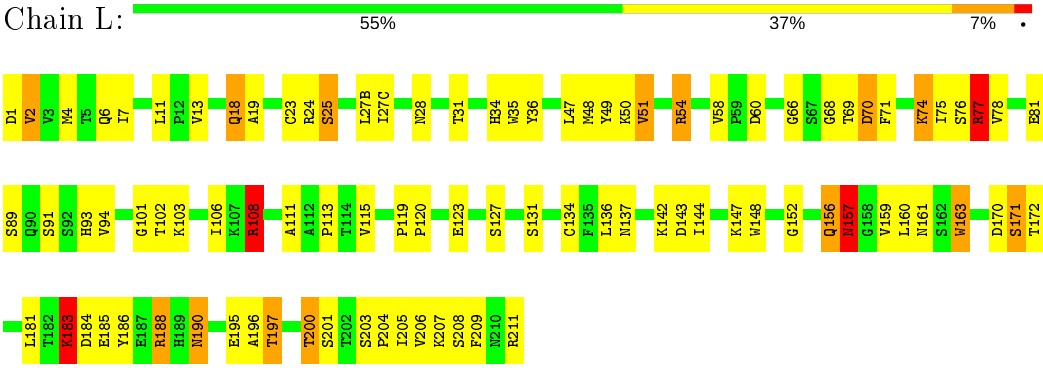
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

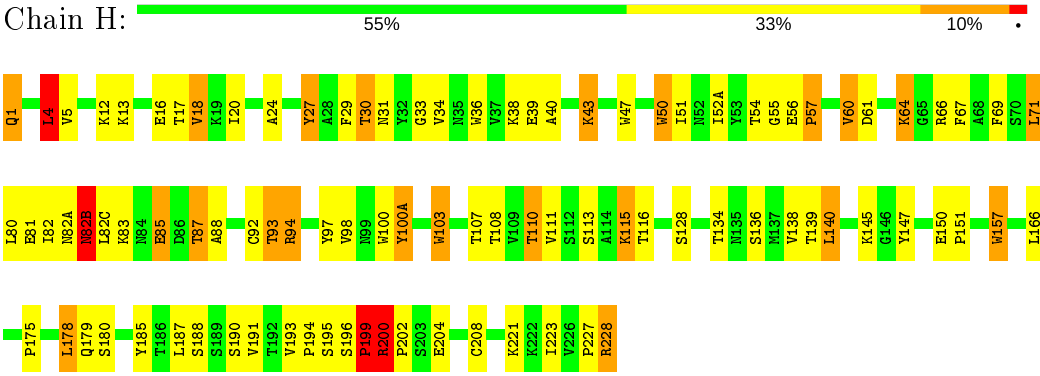
- Molecule 1: IGG1-KAPPA DB3 FAB (LIGHT CHAIN)

Chain L:



- Molecule 2: IGG1-KAPPA DB3 FAB (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	134.76Å 134.76Å 124.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.213 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3377	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	L	1.02	2/1719 (0.1%)	2.06	41/2331 (1.8%)
2	H	1.01	1/1723 (0.1%)	2.35	65/2358 (2.8%)
All	All	1.01	3/3442 (0.1%)	2.21	106/4689 (2.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	163	TRP	CG-CD2	-5.57	1.34	1.43
2	H	157	TRP	CG-CD2	-5.31	1.34	1.43
1	L	170	ASP	CB-CG	5.02	1.62	1.51

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	163	TRP	CD1-CG-CD2	18.00	120.70	106.30
1	L	148	TRP	CD1-CG-CD2	17.82	120.56	106.30
2	H	157	TRP	CD1-CG-CD2	17.79	120.53	106.30
2	H	47	TRP	CD1-CG-CD2	17.78	120.52	106.30
2	H	100	TRP	CD1-CG-CD2	17.77	120.52	106.30
2	H	50	TRP	CD1-CG-CD2	17.76	120.51	106.30
2	H	36	TRP	CD1-CG-CD2	17.74	120.49	106.30
1	L	35	TRP	CD1-CG-CD2	17.47	120.28	106.30
2	H	103	TRP	CD1-CG-CD2	17.37	120.20	106.30
2	H	200	ARG	NE-CZ-NH2	-17.05	111.78	120.30
2	H	103	TRP	CE2-CD2-CG	-14.75	95.50	107.30
2	H	200	ARG	NE-CZ-NH1	14.62	127.61	120.30
2	H	157	TRP	CE2-CD2-CG	-14.41	95.77	107.30
1	L	148	TRP	CE2-CD2-CG	-14.36	95.81	107.30
2	H	50	TRP	CE2-CD2-CG	-14.33	95.84	107.30
2	H	47	TRP	CE2-CD2-CG	-14.25	95.90	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	100	TRP	CE2-CD2-CG	-14.23	95.92	107.30
1	L	35	TRP	CE2-CD2-CG	-14.16	95.97	107.30
2	H	36	TRP	CE2-CD2-CG	-13.93	96.16	107.30
1	L	163	TRP	CE2-CD2-CG	-13.36	96.61	107.30
2	H	66	ARG	NE-CZ-NH2	-12.13	114.23	120.30
1	L	108	ARG	NE-CZ-NH2	-11.73	114.43	120.30
2	H	100(A)	TYR	CB-CG-CD2	-10.79	114.52	121.00
2	H	100(A)	TYR	CB-CG-CD1	10.77	127.46	121.00
1	L	70	ASP	CB-CG-OD2	-10.68	108.69	118.30
1	L	148	TRP	CG-CD1-NE1	-10.24	99.86	110.10
2	H	103	TRP	CG-CD2-CE3	10.22	143.10	133.90
1	L	77	ARG	NE-CZ-NH1	10.17	125.39	120.30
2	H	36	TRP	CG-CD1-NE1	-9.91	100.19	110.10
2	H	47	TRP	CG-CD1-NE1	-9.83	100.27	110.10
1	L	108	ARG	NE-CZ-NH1	9.76	125.18	120.30
2	H	100	TRP	CG-CD1-NE1	-9.67	100.43	110.10
1	L	163	TRP	CG-CD1-NE1	-9.66	100.44	110.10
2	H	157	TRP	CG-CD1-NE1	-9.63	100.47	110.10
1	L	148	TRP	CG-CD2-CE3	9.57	142.51	133.90
2	H	100	TRP	CG-CD2-CE3	9.57	142.51	133.90
1	L	35	TRP	CG-CD1-NE1	-9.51	100.59	110.10
2	H	50	TRP	CG-CD1-NE1	-9.39	100.71	110.10
2	H	157	TRP	CG-CD2-CE3	9.37	142.34	133.90
2	H	47	TRP	CG-CD2-CE3	9.34	142.31	133.90
2	H	36	TRP	CG-CD2-CE3	9.31	142.28	133.90
2	H	103	TRP	CG-CD1-NE1	-9.26	100.84	110.10
1	L	35	TRP	CG-CD2-CE3	9.16	142.14	133.90
1	L	70	ASP	CB-CG-OD1	9.06	126.45	118.30
2	H	50	TRP	CG-CD2-CE3	9.01	142.01	133.90
2	H	103	TRP	CB-CG-CD1	-8.99	115.31	127.00
1	L	148	TRP	CB-CG-CD1	-8.69	115.71	127.00
1	L	211	ARG	NE-CZ-NH2	-8.55	116.03	120.30
2	H	204	GLU	CA-CB-CG	8.32	131.71	113.40
2	H	157	TRP	CB-CG-CD1	-8.25	116.27	127.00
1	L	163	TRP	CG-CD2-CE3	8.09	141.18	133.90
1	L	211	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	H	93	THR	CA-CB-CG2	-7.68	101.64	112.40
2	H	1	GLN	N-CA-C	-7.51	90.71	111.00
2	H	193	VAL	CG1-CB-CG2	-7.46	98.97	110.90
2	H	147	TYR	CB-CG-CD2	-7.37	116.58	121.00
2	H	47	TRP	CB-CG-CD1	-7.33	117.47	127.00
2	H	147	TYR	CB-CG-CD1	7.22	125.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	100	TRP	CB-CG-CD1	-7.14	117.72	127.00
2	H	36	TRP	CB-CG-CD1	-6.96	117.96	127.00
1	L	152	GLY	N-CA-C	-6.82	96.05	113.10
1	L	211	ARG	CA-CB-CG	6.78	128.32	113.40
2	H	178	LEU	CA-CB-CG	6.64	130.57	115.30
2	H	134	THR	O-C-N	-6.63	112.09	122.70
2	H	66	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	L	203	SER	N-CA-C	-6.55	93.32	111.00
2	H	200	ARG	CA-CB-CG	-6.52	99.05	113.40
2	H	199	PRO	CA-N-CD	-6.39	102.56	111.50
2	H	94	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	H	134	THR	CA-C-N	6.27	131.00	117.20
1	L	163	TRP	CB-CG-CD2	-6.25	118.47	126.60
2	H	166	LEU	N-CA-C	-6.14	94.41	111.00
2	H	187	LEU	CA-CB-CG	6.14	129.41	115.30
1	L	170	ASP	CB-CG-OD1	6.11	123.80	118.30
2	H	228	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	H	199	PRO	CA-C-N	-6.02	103.95	117.20
1	L	142	LYS	CA-C-N	5.89	130.16	117.20
1	L	171	SER	N-CA-C	5.87	126.86	111.00
2	H	60	VAL	N-CA-C	-5.86	95.18	111.00
1	L	35	TRP	CB-CG-CD2	-5.85	118.99	126.60
1	L	51	VAL	CA-C-N	5.82	130.01	117.20
1	L	142	LYS	CA-CB-CG	5.74	126.03	113.40
2	H	85	GLU	CA-CB-CG	5.73	126.02	113.40
1	L	35	TRP	NE1-CE2-CD2	5.70	113.00	107.30
2	H	103	TRP	NE1-CE2-CD2	5.69	112.99	107.30
2	H	145	LYS	CA-CB-CG	5.64	125.81	113.40
2	H	82(B)	ASN	CA-C-N	-5.61	104.86	117.20
1	L	102	THR	OG1-CB-CG2	-5.60	97.12	110.00
1	L	54	ARG	CA-CB-CG	5.60	125.72	113.40
1	L	51	VAL	CG1-CB-CG2	-5.53	102.06	110.90
2	H	50	TRP	CB-CG-CD1	-5.48	119.88	127.00
1	L	143	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	L	190	ASN	CA-C-N	5.42	129.14	117.20
2	H	50	TRP	CB-CG-CD2	-5.39	119.60	126.60
1	L	183	LYS	CA-CB-CG	5.36	125.19	113.40
2	H	194	PRO	CA-N-CD	-5.33	104.04	111.50
2	H	64	LYS	CA-CB-CG	5.32	125.09	113.40
2	H	50	TRP	NE1-CE2-CD2	5.31	112.61	107.30
1	L	74	LYS	CA-CB-CG	5.30	125.06	113.40
1	L	54	ARG	NE-CZ-NH1	5.25	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	98	VAL	CG1-CB-CG2	-5.23	102.53	110.90
2	H	134	THR	N-CA-C	-5.19	96.99	111.00
2	H	4	LEU	N-CA-C	-5.15	97.09	111.00
1	L	108	ARG	CA-C-N	-5.14	105.88	117.20
2	H	38	LYS	CA-CB-CG	5.11	124.64	113.40
1	L	157	ASN	N-CA-C	5.04	124.60	111.00

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	L	1679	0	1625	42	0
2	H	1675	0	1633	44	0
3	H	21	0	28	1	0
4	H	1	0	0	0	0
4	L	1	0	0	0	0
All	All	3377	0	3286	84	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 13.

All (84) 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:L:160:LEU:HD11	2:H:179:GLN:HB3	1.61	0.83
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.66	0.77
1:L:159:VAL:HB	1:L:161:ASN:HD21	1.50	0.77
2:H:93:THR:HG22	2:H:103:TRP:HA	1.67	0.77
1:L:108:ARG:NH2	1:L:111:ALA:HB2	2.01	0.76
2:H:51:ILE:HD13	2:H:71:LEU:HD23	1.70	0.72
1:L:115:VAL:HG13	1:L:207:LYS:HD2	1.71	0.72
2:H:34:VAL:HG22	2:H:51:ILE:HG22	1.71	0.72
1:L:159:VAL:HB	1:L:161:ASN:ND2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:GLU:HG3	2:H:17:THR:N	2.11	0.66
2:H:17:THR:HG22	2:H:82(B):ASN:H	1.61	0.65
1:L:163:TRP:HZ3	1:L:173:TYR:HB3	1.63	0.62
2:H:12:LYS:O	2:H:111:VAL:HA	2.00	0.61
2:H:24:ALA:HB1	2:H:27:TYR:CE2	2.35	0.61
2:H:16:GLU:HG3	2:H:17:THR:H	1.67	0.59
2:H:33:GLY:HA3	2:H:50:TRP:HE1	1.67	0.59
2:H:27:TYR:CE1	2:H:29:PHE:HA	2.37	0.58
1:L:156:GLN:HB2	1:L:157:ASN:OD1	2.03	0.58
1:L:108:ARG:HH22	1:L:111:ALA:HB2	1.69	0.57
2:H:93:THR:HG21	2:H:103:TRP:CD2	2.39	0.57
1:L:47:LEU:O	1:L:58:VAL:HG21	2.05	0.57
1:L:147:LYS:HB3	1:L:195:GLU:HB3	1.86	0.56
1:L:159:VAL:O	1:L:160:LEU:HD23	2.05	0.56
1:L:163:TRP:CZ3	1:L:173:TYR:HB3	2.41	0.55
2:H:17:THR:HB	2:H:82(A):ASN:HA	1.88	0.55
1:L:25:SER:O	1:L:69:THR:HG23	2.06	0.55
1:L:197:THR:HG23	1:L:204:PRO:HB3	1.90	0.54
1:L:34:HIS:HE1	1:L:91:SER:OG	1.90	0.53
2:H:18:VAL:O	2:H:81:GLU:HA	2.09	0.53
2:H:20:ILE:HG12	2:H:107:THR:HG21	1.90	0.53
1:L:175:MET:HG2	1:L:176:SER:N	2.25	0.52
2:H:171:VAL:HA	2:H:190:SER:O	2.10	0.51
2:H:67:PHE:CE2	2:H:82:ILE:HG12	2.45	0.51
2:H:18:VAL:HG22	2:H:82(C):LEU:HD11	1.93	0.51
1:L:86:TYR:O	1:L:101:GLY:HA2	2.12	0.50
1:L:94:VAL:HG13	3:H:229:ANO:H22	1.91	0.50
2:H:196:SER:HB2	2:H:199:PRO:HD3	1.92	0.50
1:L:25:SER:OG	1:L:69:THR:HA	2.12	0.48
2:H:54:THR:HG23	2:H:56:GLU:H	1.78	0.48
2:H:51:ILE:HG13	2:H:57:PRO:HG3	1.95	0.48
2:H:30:THR:HA	2:H:52(A):ILE:HG22	1.94	0.48
1:L:195:GLU:HG3	1:L:206:VAL:CG1	2.44	0.48
1:L:18:GLN:HA	1:L:76:SER:O	2.14	0.47
1:L:2:VAL:HG21	1:L:93:HIS:HD2	1.77	0.47
2:H:51:ILE:HD12	2:H:69:PHE:HB3	1.97	0.47
1:L:136:LEU:HD21	1:L:196:ALA:HB2	1.96	0.47
1:L:4:MET:HE3	1:L:23:CYS:SG	2.55	0.47
2:H:12:LYS:CE	2:H:16:GLU:HG2	2.45	0.46
2:H:39:GLU:O	2:H:88:ALA:HB1	2.14	0.46
1:L:19:ALA:HB3	1:L:75:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:119:PRO:HB3	1:L:209:PHE:CZ	2.51	0.46
2:H:140:LEU:HB3	2:H:223:ILE:HG21	1.98	0.46
2:H:139:THR:HA	2:H:191:VAL:O	2.16	0.45
2:H:202:PRO:HB3	2:H:227:PRO:HD3	1.98	0.45
2:H:178:LEU:HB3	2:H:185:TYR:CD1	2.52	0.45
1:L:82:ASP:HB3	1:L:86:TYR:OH	2.17	0.44
1:L:47:LEU:HD23	1:L:58:VAL:HG22	1.98	0.44
2:H:33:GLY:HA3	2:H:50:TRP:NE1	2.33	0.44
2:H:93:THR:CG2	2:H:103:TRP:HA	2.45	0.44
2:H:4:LEU:HG	2:H:92:CYS:SG	2.58	0.43
2:H:67:PHE:HD2	2:H:80:LEU:HD11	1.83	0.43
1:L:113:PRO:HA	1:L:137:ASN:O	2.18	0.43
1:L:27(B):LEU:HD12	1:L:71:PHE:CZ	2.53	0.43
1:L:36:TYR:HE2	1:L:89:SER:OG	2.02	0.43
1:L:181:LEU:HD13	1:L:186:TYR:HB2	2.00	0.43
1:L:77:ARG:HB2	1:L:77:ARG:HH11	1.83	0.43
1:L:115:VAL:HG23	1:L:134:CYS:SG	2.59	0.42
2:H:12:LYS:HE3	2:H:16:GLU:HG2	2.00	0.42
1:L:123:GLU:HG2	2:H:221:LYS:NZ	2.35	0.42
2:H:157:TRP:CZ3	2:H:208:CYS:HB3	2.55	0.42
2:H:55:GLY:O	2:H:57:PRO:HD3	2.19	0.42
1:L:27(B):LEU:O	1:L:31:THR:HA	2.18	0.42
1:L:66:GLY:HA3	1:L:70:ASP:O	2.20	0.42
2:H:200:ARG:HG2	2:H:202:PRO:HA	2.01	0.42
1:L:13:VAL:HG11	1:L:78:VAL:HG21	2.02	0.42
2:H:87:THR:HG23	2:H:110:THR:HA	2.01	0.41
1:L:120:PRO:HG3	1:L:131:SER:O	2.21	0.41
2:H:196:SER:HB2	2:H:199:PRO:CD	2.50	0.41
2:H:115:LYS:HE2	2:H:116:THR:H	1.85	0.41
1:L:185:GLU:O	1:L:188:ARG:HG3	2.20	0.41
1:L:183:LYS:O	1:L:186:TYR:HB3	2.21	0.41
1:L:136:LEU:HD22	1:L:144:ILE:HD11	2.04	0.40
2:H:34:VAL:HG13	2:H:52(A):ILE:HD11	2.03	0.40
2:H:33:GLY:O	2:H:94:ARG:HA	2.20	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	L	214/216 (99%)	181 (85%)	26 (12%)	7 (3%)	4 21
2	H	217/219 (99%)	192 (88%)	20 (9%)	5 (2%)	6 30
All	All	431/435 (99%)	373 (86%)	46 (11%)	12 (3%)	5 25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	2	VAL
2	H	87	THR
2	H	136	SER
2	H	199	PRO
1	L	51	VAL
1	L	200	THR
2	H	97	TYR
1	L	50	LYS
1	L	68	GLY
1	L	157	ASN
1	L	171	SER
2	H	82(B)	ASN

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	L	194/194 (100%)	162 (84%)	32 (16%)	2 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	188/188 (100%)	153 (81%)	35 (19%)	1 8
All	All	382/382 (100%)	315 (82%)	67 (18%)	2 10

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	6	GLN
1	L	7	ILE
1	L	11	LEU
1	L	18	GLN
1	L	24	ARG
1	L	25	SER
1	L	27(C)	ILE
1	L	28	ASN
1	L	48	MET
1	L	49	TYR
1	L	54	ARG
1	L	60	ASP
1	L	74	LYS
1	L	77	ARG
1	L	81	GLU
1	L	82	ASP
1	L	103	LYS
1	L	106	ILE
1	L	108	ARG
1	L	127	SER
1	L	156	GLN
1	L	172	THR
1	L	183	LYS
1	L	184	ASP
1	L	188	ARG
1	L	190	ASN
1	L	197	THR
1	L	200	THR
1	L	201	SER
1	L	205	ILE
1	L	208	SER
2	H	1	GLN
2	H	4	LEU
2	H	5	VAL
2	H	13	LYS

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Mol	Chain	Res	Type
2	H	18	VAL
2	H	27	TYR
2	H	30	THR
2	H	31	ASN
2	H	43	LYS
2	H	57	PRO
2	H	60	VAL
2	H	61	ASP
2	H	64	LYS
2	H	71	LEU
2	H	73	THR
2	H	74	SER
2	H	83	LYS
2	H	85	GLU
2	H	100(A)	TYR
2	H	108	THR
2	H	110	THR
2	H	113	SER
2	H	115	LYS
2	H	128	SER
2	H	138	VAL
2	H	140	LEU
2	H	150	GLU
2	H	151	PRO
2	H	168	SER
2	H	175	PRO
2	H	180	SER
2	H	188	SER
2	H	195	SER
2	H	200	ARG
2	H	228	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	34	HIS
1	L	38	GLN
1	L	137	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 carbohydrates 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	ANO	H	229	-	24,24,24	1.23	3 (12%)	39,39,39	2.58	19 (48%)

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	ANO	H	229	-	-	-	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	229	ANO	C12-C13	-2.76	1.49	1.54
3	H	229	ANO	C16-C17	2.09	1.54	1.51
3	H	229	ANO	C4-C3	2.07	1.54	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	229	ANO	C14-C13-C17	-4.82	95.06	100.59
3	H	229	ANO	C5-C4-C3	4.54	120.95	112.73
3	H	229	ANO	C1-C2-C3	4.49	121.26	111.95
3	H	229	ANO	C12-C13-C14	4.43	115.98	108.99
3	H	229	ANO	C6-C5-C4	-4.33	105.01	111.11
3	H	229	ANO	C2-C3-C4	-3.98	109.96	115.89
3	H	229	ANO	C4-C5-C10	-3.97	109.04	112.79
3	H	229	ANO	C10-C9-C8	-3.48	108.77	112.42
3	H	229	ANO	C13-C14-C8	-3.48	109.40	113.12
3	H	229	ANO	C18-C13-C12	-3.26	107.30	111.13
3	H	229	ANO	C1-C10-C9	3.20	116.39	111.35
3	H	229	ANO	C19-C10-C9	-3.16	106.83	111.18
3	H	229	ANO	C15-C14-C8	2.77	123.64	119.08
3	H	229	ANO	C18-C13-C14	2.69	116.95	112.98
3	H	229	ANO	C11-C9-C10	-2.65	110.86	113.91
3	H	229	ANO	C12-C13-C17	-2.48	112.95	116.67
3	H	229	ANO	C11-C12-C13	-2.47	107.39	112.74
3	H	229	ANO	C2-C1-C10	2.36	116.50	113.47
3	H	229	ANO	O3-C3-C2	2.28	125.93	122.05

There are no chirality outliers.

There are no torsion outliers.

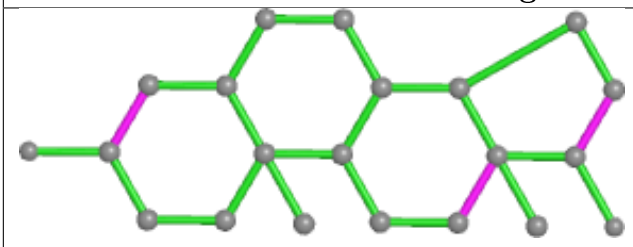
There are no ring outliers.

1 monomer is involved in 1 short contact:

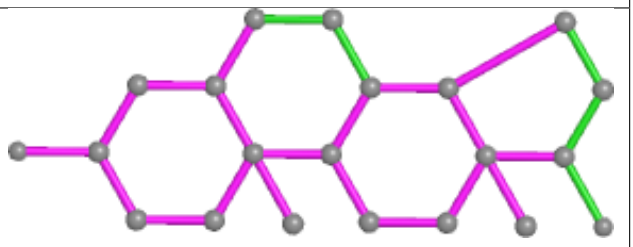
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	229	ANO	1	0

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 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.

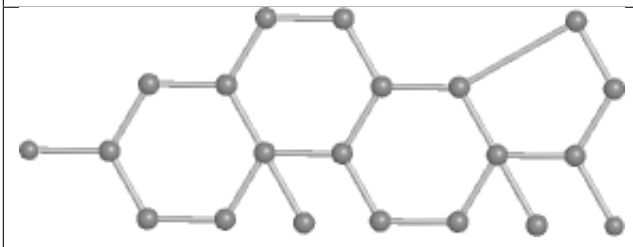
Ligand ANO H 229



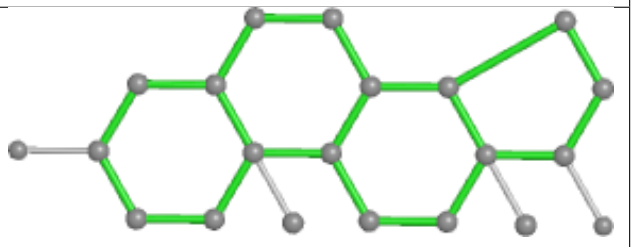
Bond lengths



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.