Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2024 – 06:04 AM EDT

PDB ID	:	1IND
Title	:	HOW THE ANTI-(METAL CHELATE) ANTIBODY CHA255 IS SPECIFIC FOR THE METAL ION OF ITS ANTIGEN: X-RAY STRUCTURES FOR TWO FAB'(SLASH)HAPTEN COMPLEXES WITH DIFFERENT METALS IN THE CHELATE
Authors	:	Love, R.A.; Butler, W.F.
Deposited on	:	1993-06-14
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

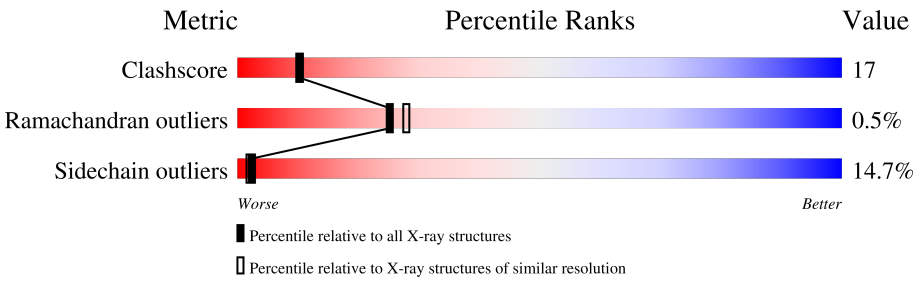
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.20 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))
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	215	55% 34% 7% • •
2	H	226	50% 33% 9% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3374 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-LAMBDA CHA255 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1601	1002	270	323	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	87	ARG	ILE	conflict	GB 387376
L	97	LEU	HIS	conflict	GB 387376
L	140	ILE	THR	conflict	GB 387376
L	187	GLU	ALA	conflict	GB 387376

- Molecule 2 is a protein called IGG1-LAMBDA CHA255 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	213	1593	1004	271	312	6	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	3	THR	LYS	conflict	PIR S38864
H	5	VAL	LEU	conflict	PIR S38864
H	11	SER	LEU	conflict	PIR S38864
H	27	PHE	LEU	conflict	PIR S38864
H	29	LEU	PHE	conflict	PIR S38864
H	31	GLY	SER	conflict	PIR S38864
H	32	GLU	TYR	conflict	PIR S38864
H	33	THR	GLY	conflict	PIR S38864
H	40	THR	ILE	conflict	PIR S38864
H	42	GLU	ASP	conflict	PIR S38864
H	51	THR	ILE	conflict	PIR S38864
H	52	LEU	SER	conflict	PIR S38864

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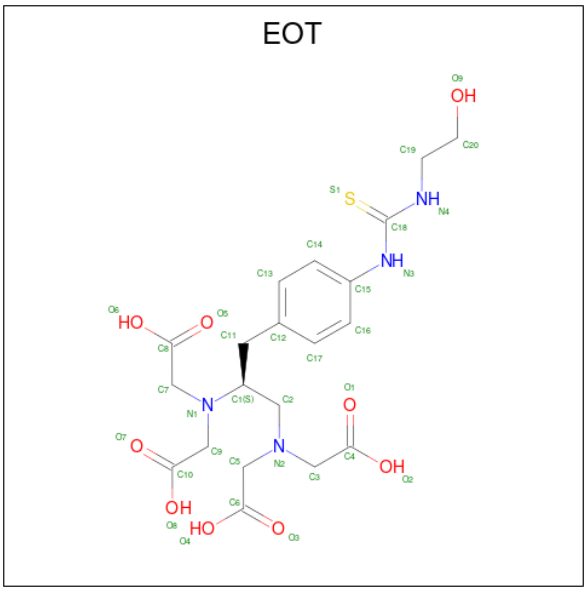
Chain	Residue	Modelled	Actual	Comment	Reference
H	56	GLY	THR	conflict	PIR S38864
H	57	PHE	TYR	conflict	PIR S38864
H	59	PHE	TYR	conflict	PIR S38864
H	61	SER	PRO	conflict	PIR S38864
H	62	ALA	ASP	conflict	PIR S38864
H	76	GLN	LYS	conflict	PIR S38864
H	78	ASN	THR	conflict	PIR S38864
H	83	LEU	MET	conflict	PIR S38864
H	84	ASN	SER	conflict	PIR S38864
H	87	ARG	LYS	conflict	PIR S38864
H	93	LEU	MET	conflict	PIR S38864
H	95	PHE	TYR	conflict	PIR S38864
H	?	-	ARG	deletion	PIR S38864
H	?	-	GLN	deletion	PIR S38864
H	?	-	GLY	deletion	PIR S38864
H	?	-	VAL	deletion	PIR S38864
H	?	-	THR	deletion	PIR S38864
H	?	-	MET	deletion	PIR S38864
H	99	HIS	ILE	conflict	PIR S38864
H	102	VAL	ALA	conflict	PIR S38864
H	103	HIS	TYR	conflict	PIR S38864
H	106	HIS	GLN	conflict	PIR S38864
H	?	-	GLY	deletion	PIR S38864
H	171	GLU	GLN	conflict	PIR S38864
H	187	PRO	THR	conflict	PIR S38864
H	188	ARG	TRP	conflict	PIR S38864
H	222	CYS	-	insertion	PIR S38864
H	223	THR	-	insertion	PIR S38864

- Molecule 3 is INDIUM (III) ION (three-letter code: IN) (formula: In).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	In		
3	H	1	1	1	0	0

- Molecule 4 is [(1-[(BIS-CARBOXYMETHYL-AMINO)-METHYL]-2-{4-[3-(2-HYDROXY-ETHYL)-THIOUREIDO]-PHENY}-ETHYL)-CARBOXYMETHYL-AMINO]-ACETIC ACID (three-letter code: EOT) (formula: $C_{20}H_{28}N_4O_9S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	H	1	34	20	4	9	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	L	69	69	69	0	0
			Total	O		
5	H	76	76	76	0	0

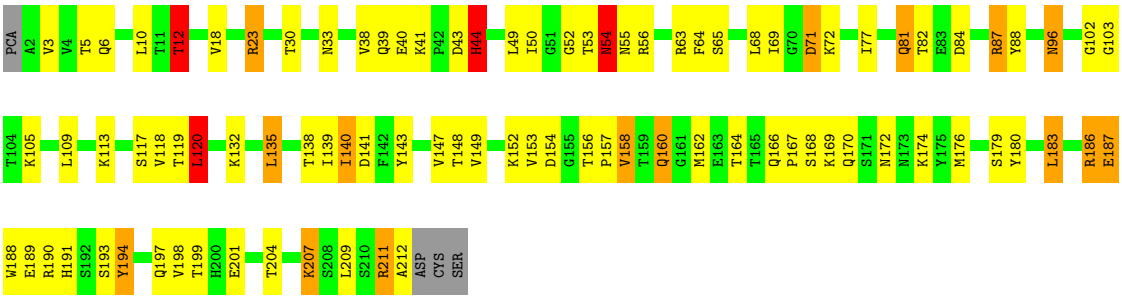
3 Residue-property plots (i)

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. 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.

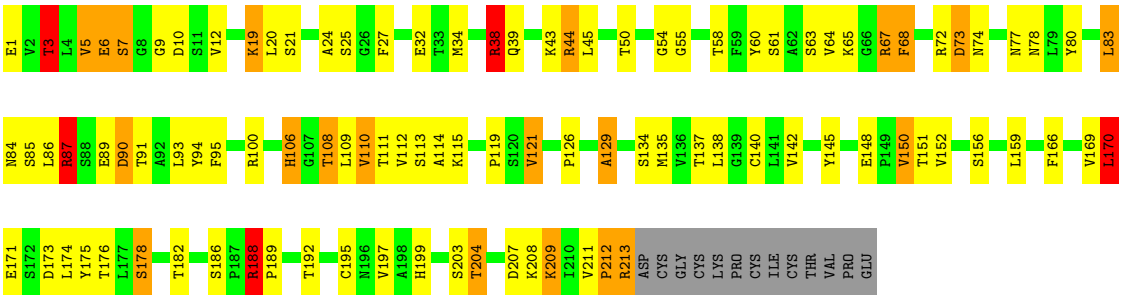
- Molecule 1: IGG1-LAMBDA CHA255 FAB (LIGHT CHAIN)

Chain L:



- Molecule 2: IGG1-LAMBDA CHA255 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	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.30Å 84.60Å 76.70Å 90.00° 136.20° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, TNT, X-PLOR	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3374	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

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: IN, EOT

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	0.99	0/1638	2.03	48/2238 (2.1%)
2	H	1.03	0/1633	2.11	61/2231 (2.7%)
All	All	1.01	0/3271	2.07	109/4469 (2.4%)

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
2	H	0	1

There are no bond length outliers.

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	67	ARG	NE-CZ-NH2	-18.00	111.30	120.30
2	H	67	ARG	NE-CZ-NH1	15.20	127.90	120.30
1	L	63	ARG	CD-NE-CZ	15.18	144.85	123.60
1	L	63	ARG	NE-CZ-NH2	14.77	127.68	120.30
2	H	213	ARG	NE-CZ-NH1	14.73	127.67	120.30
1	L	87	ARG	NE-CZ-NH1	14.58	127.59	120.30
1	L	56	ARG	NE-CZ-NH1	12.56	126.58	120.30
2	H	38	ARG	NE-CZ-NH2	-12.37	114.11	120.30
1	L	211	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	L	87	ARG	NE-CZ-NH2	-11.20	114.70	120.30
2	H	38	ARG	CD-NE-CZ	10.21	137.89	123.60
1	L	87	ARG	CD-NE-CZ	9.79	137.31	123.60
2	H	188	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	L	190	ARG	NE-CZ-NH1	9.44	125.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	71	ASP	CB-CG-OD1	9.43	126.78	118.30
1	L	63	ARG	CA-CB-CG	9.20	133.63	113.40
2	H	10	ASP	CB-CG-OD1	9.19	126.57	118.30
1	L	135	LEU	CA-CB-CG	9.12	136.27	115.30
2	H	87	ARG	NE-CZ-NH1	8.95	124.78	120.30
2	H	186	SER	CB-CA-C	8.93	127.07	110.10
1	L	43	ASP	CB-CG-OD1	8.72	126.15	118.30
2	H	67	ARG	CD-NE-CZ	8.64	135.69	123.60
2	H	44	ARG	NE-CZ-NH1	8.56	124.58	120.30
2	H	83	LEU	CA-CB-CG	8.44	134.72	115.30
2	H	213	ARG	CD-NE-CZ	8.11	134.95	123.60
2	H	213	ARG	NE-CZ-NH2	-7.95	116.32	120.30
2	H	54	GLY	N-CA-C	-7.91	93.32	113.10
2	H	150	VAL	CA-CB-CG1	7.87	122.70	110.90
1	L	186	ARG	NE-CZ-NH2	7.68	124.14	120.30
2	H	3	THR	CA-CB-CG2	7.63	123.08	112.40
2	H	90	ASP	CB-CG-OD1	7.55	125.10	118.30
2	H	72	ARG	CD-NE-CZ	7.46	134.05	123.60
2	H	72	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	L	183	LEU	CA-CB-CG	7.18	131.82	115.30
2	H	188	ARG	CD-NE-CZ	7.17	133.64	123.60
2	H	100	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	L	119	THR	CA-CB-CG2	7.10	122.34	112.40
2	H	84	ASN	N-CA-C	6.99	129.88	111.00
2	H	170	LEU	CA-CB-CG	6.87	131.11	115.30
2	H	114	ALA	CA-C-N	6.87	132.31	117.20
1	L	84	ASP	CB-CG-OD1	6.81	124.43	118.30
1	L	23	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	L	12	THR	N-CA-CB	6.78	123.17	110.30
1	L	63	ARG	NE-CZ-NH1	-6.75	116.93	120.30
2	H	38	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	L	105	LYS	CA-CB-CG	6.55	127.82	113.40
2	H	174	LEU	CA-CB-CG	6.54	130.33	115.30
2	H	108	THR	N-CA-CB	6.49	122.64	110.30
1	L	23	ARG	CD-NE-CZ	6.45	132.64	123.60
1	L	44	HIS	CA-CB-CG	6.44	124.55	113.60
1	L	154	ASP	CB-CG-OD1	6.39	124.05	118.30
1	L	53	THR	O-C-N	-6.37	112.52	122.70
2	H	20	LEU	CA-CB-CG	6.24	129.65	115.30
1	L	207	LYS	N-CA-CB	6.20	121.76	110.60
2	H	44	ARG	CD-NE-CZ	6.20	132.28	123.60
2	H	113	SER	N-CA-CB	-6.14	101.29	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	186	ARG	NH1-CZ-NH2	-6.13	112.65	119.40
1	L	190	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	L	158	VAL	CA-CB-CG1	5.97	119.86	110.90
2	H	45	LEU	CA-CB-CG	5.97	129.02	115.30
2	H	64	VAL	CA-CB-CG1	5.96	119.85	110.90
2	H	195	CYS	N-CA-CB	5.94	121.28	110.60
1	L	68	LEU	CA-CB-CG	5.92	128.92	115.30
2	H	10	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	L	54	ASN	N-CA-CB	5.86	121.15	110.60
1	L	71	ASP	CB-CA-C	5.86	122.11	110.40
2	H	169	VAL	CA-CB-CG1	5.86	119.68	110.90
1	L	186	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	L	3	VAL	CA-CB-CG2	5.75	119.52	110.90
1	L	190	ARG	CD-NE-CZ	5.74	131.64	123.60
1	L	211	ARG	CD-NE-CZ	5.74	131.63	123.60
2	H	137	THR	CA-CB-CG2	5.73	120.43	112.40
2	H	110	VAL	CA-CB-CG2	5.71	119.46	110.90
2	H	19	LYS	CB-CA-C	5.63	121.65	110.40
2	H	50	THR	CA-CB-CG2	5.62	120.27	112.40
1	L	158	VAL	CB-CA-C	5.58	121.99	111.40
2	H	114	ALA	CA-C-O	-5.57	108.41	120.10
2	H	83	LEU	CB-CA-C	5.56	120.76	110.20
1	L	71	ASP	CA-CB-CG	5.52	125.55	113.40
2	H	64	VAL	N-CA-CB	-5.48	99.44	111.50
2	H	159	LEU	CB-CA-C	5.45	120.56	110.20
2	H	68	PHE	CB-CG-CD1	5.44	124.61	120.80
2	H	85	SER	N-CA-C	-5.41	96.41	111.00
2	H	176	THR	CA-CB-CG2	5.40	119.96	112.40
1	L	56	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	L	56	ARG	CG-CD-NE	5.39	123.12	111.80
2	H	44	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	L	81	GLN	CB-CG-CD	5.33	125.45	111.60
1	L	120	LEU	CA-CB-CG	5.31	127.51	115.30
2	H	87	ARG	CG-CD-NE	5.30	122.92	111.80
2	H	204	THR	CA-CB-CG2	5.25	119.75	112.40
2	H	68	PHE	CA-CB-CG	5.24	126.48	113.90
2	H	207	ASP	CB-CG-OD2	5.23	123.01	118.30
2	H	19	LYS	CA-CB-CG	5.22	124.89	113.40
2	H	121	VAL	CA-CB-CG1	5.22	118.72	110.90
2	H	89	GLU	CA-CB-CG	5.18	124.80	113.40
1	L	186	ARG	CD-NE-CZ	5.18	130.85	123.60
2	H	110	VAL	N-CA-CB	5.17	122.87	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	10	LEU	CA-C-N	-5.15	105.88	117.20
1	L	211	ARG	NE-CZ-NH2	-5.15	117.73	120.30
2	H	73	ASP	CB-CG-OD2	-5.14	113.67	118.30
2	H	129	ALA	C-N-CA	5.14	134.56	121.70
1	L	40	GLU	CA-CB-CG	5.13	124.68	113.40
1	L	194	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	L	84	ASP	CB-CG-OD2	-5.06	113.74	118.30
2	H	173	ASP	CB-CG-OD2	-5.05	113.75	118.30
2	H	55	GLY	C-N-CA	5.03	132.86	122.30
1	L	160	GLN	CA-CB-CG	5.02	124.45	113.40
2	H	209	LYS	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	38	ARG	Sidechain

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	1601	0	1550	56	0
2	H	1593	0	1570	54	0
3	H	1	0	0	0	0
4	H	34	0	24	0	0
5	H	76	0	0	8	0
5	L	69	0	0	7	0
All	All	3374	0	3144	107	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 17.

All (107) 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:H:3:THR:HG22	2:H:25:SER:HB2	1.29	1.07
1:L:153:VAL:CG2	1:L:158:VAL:HG21	2.00	0.92
2:H:32:GLU:HG2	2:H:34:MET:HE2	1.51	0.90
1:L:164:THR:CG2	5:L:396:HOH:O	2.19	0.89
2:H:3:THR:HG22	2:H:25:SER:CB	2.01	0.89
1:L:39:GLN:HB2	1:L:49:LEU:HD11	1.55	0.87
1:L:30:THR:H	1:L:33:ASN:HD22	1.21	0.87
2:H:188:ARG:HD2	2:H:189:PRO:HA	1.57	0.86
2:H:74:ASN:O	5:H:334:HOH:O	1.98	0.81
1:L:164:THR:HG22	5:L:396:HOH:O	1.81	0.81
2:H:121:VAL:HG21	2:H:197:VAL:HG11	1.61	0.81
2:H:32:GLU:HG2	2:H:34:MET:CE	2.11	0.79
2:H:126:PRO:HB2	2:H:129:ALA:HB2	1.65	0.77
2:H:209:LYS:HD2	5:H:323:HOH:O	1.86	0.76
1:L:140:ILE:HD11	2:H:166:PHE:HZ	1.52	0.75
2:H:142:VAL:HG11	2:H:150:VAL:HG11	1.70	0.72
1:L:153:VAL:HG23	1:L:158:VAL:HG21	1.72	0.69
1:L:149:VAL:HG22	1:L:198:VAL:HG22	1.75	0.69
2:H:138:LEU:HD11	2:H:188:ARG:HG3	1.75	0.68
1:L:140:ILE:HG23	1:L:141:ASP:OD1	1.95	0.67
1:L:212:ALA:HA	5:L:339:HOH:O	1.95	0.67
1:L:153:VAL:HB	1:L:158:VAL:CG2	2.26	0.66
1:L:30:THR:H	1:L:33:ASN:ND2	1.91	0.66
2:H:121:VAL:HG12	2:H:208:LYS:HG3	1.79	0.65
2:H:60:TYR:HB2	2:H:65:LYS:HD2	1.78	0.64
1:L:153:VAL:CB	1:L:158:VAL:HG21	2.27	0.64
2:H:74:ASN:HA	5:H:334:HOH:O	1.97	0.63
1:L:120:LEU:HD13	1:L:209:LEU:HD23	1.81	0.63
2:H:5:VAL:HG23	2:H:106:HIS:CE1	2.34	0.63
1:L:153:VAL:HB	1:L:158:VAL:HG21	1.81	0.62
1:L:5:THR:HG22	1:L:23:ARG:HB3	1.80	0.62
2:H:121:VAL:CG2	2:H:197:VAL:HG11	2.30	0.62
2:H:91:THR:HG23	2:H:111:THR:HA	1.82	0.61
2:H:152:VAL:HG22	2:H:197:VAL:HG23	1.82	0.61
2:H:7:SER:HA	2:H:108:THR:HG21	1.83	0.61
1:L:199:THR:HG22	1:L:204:THR:HG23	1.83	0.60
1:L:199:THR:HG23	5:L:408:HOH:O	2.01	0.60
2:H:121:VAL:HG21	2:H:197:VAL:CG1	2.31	0.59
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.84	0.59
1:L:118:VAL:HG22	1:L:139:ILE:HG23	1.87	0.57
1:L:23:ARG:HB2	1:L:72:LYS:HE3	1.87	0.57
1:L:39:GLN:NE2	1:L:41:LYS:HE3	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:PHE:CZ	2:H:34:MET:HE1	2.41	0.55
2:H:74:ASN:CA	5:H:334:HOH:O	2.55	0.55
1:L:23:ARG:NH2	5:L:306:HOH:O	2.38	0.55
2:H:27:PHE:CE2	2:H:34:MET:CE	2.91	0.53
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.40	0.53
1:L:139:ILE:HG12	1:L:198:VAL:HG21	1.90	0.53
1:L:183:LEU:HD22	1:L:187:GLU:HG2	1.91	0.52
2:H:27:PHE:CE2	2:H:34:MET:HE3	2.45	0.52
1:L:82:THR:HG23	5:L:371:HOH:O	2.09	0.52
1:L:138:THR:CG2	5:H:393:HOH:O	2.58	0.52
1:L:152:LYS:HE2	1:L:197:GLN:OE1	2.10	0.51
1:L:180:TYR:OH	2:H:178:SER:HB2	2.10	0.51
2:H:73:ASP:HB2	2:H:80:TYR:CE2	2.45	0.51
1:L:87:ARG:NH2	1:L:102:GLY:O	2.44	0.50
1:L:117:SER:HB2	1:L:140:ILE:HG22	1.92	0.50
2:H:109:LEU:HD11	5:H:361:HOH:O	2.11	0.50
2:H:93:LEU:HD23	2:H:95:PHE:CZ	2.47	0.50
1:L:44:HIS:CD2	2:H:39:GLN:HE22	2.30	0.50
1:L:50:ILE:HA	1:L:55:ASN:O	2.13	0.49
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.93	0.49
1:L:170:GLN:HE21	1:L:176:MET:HB3	1.78	0.49
1:L:109:LEU:HD13	1:L:143:TYR:HE2	1.78	0.49
1:L:191:HIS:O	1:L:211:ARG:NH1	2.46	0.48
2:H:170:LEU:HG	2:H:175:TYR:CE1	2.49	0.48
1:L:191:HIS:HB2	1:L:194:TYR:OH	2.13	0.48
2:H:135:MET:HG3	2:H:182:THR:HG22	1.96	0.47
1:L:164:THR:HG23	1:L:179:SER:HB2	1.96	0.47
1:L:135:LEU:HD11	1:L:188:TRP:HZ3	1.79	0.47
2:H:67:ARG:NH2	2:H:87:ARG:HD3	2.30	0.47
2:H:7:SER:CA	2:H:108:THR:HG21	2.45	0.46
2:H:94:TYR:CE1	2:H:110:VAL:HG22	2.51	0.46
1:L:167:PRO:HA	1:L:176:MET:O	2.16	0.46
2:H:199:HIS:HB3	2:H:204:THR:HB	1.98	0.45
1:L:162:MET:HA	1:L:180:TYR:O	2.15	0.45
1:L:189:GLU:O	1:L:211:ARG:NH1	2.50	0.45
2:H:121:VAL:O	2:H:208:LYS:HE2	2.16	0.45
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.50	0.45
2:H:73:ASP:HB2	2:H:80:TYR:HE2	1.81	0.45
1:L:148:THR:HB	1:L:199:THR:OG1	2.17	0.44
2:H:12:VAL:O	2:H:112:VAL:HA	2.18	0.44
2:H:27:PHE:CE2	2:H:34:MET:HE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:VAL:HG13	2:H:197:VAL:CG2	2.48	0.44
1:L:64:PHE:CD2	1:L:77:ILE:HG12	2.53	0.44
2:H:27:PHE:HE2	2:H:34:MET:HE3	1.83	0.44
1:L:109:LEU:HD13	1:L:143:TYR:CE2	2.53	0.43
1:L:118:VAL:HA	1:L:138:THR:O	2.18	0.43
2:H:6:GLU:HA	2:H:21:SER:O	2.19	0.43
1:L:199:THR:HG22	1:L:204:THR:CG2	2.47	0.43
2:H:211:VAL:HA	2:H:212:PRO:HD3	1.84	0.43
2:H:9:GLY:HA2	2:H:110:VAL:HG12	2.00	0.43
2:H:1:GLU:HG3	5:H:404:HOH:O	2.18	0.43
2:H:150:VAL:HG13	2:H:197:VAL:HG22	2.01	0.42
1:L:172:ASN:ND2	1:L:174:LYS:HD2	2.34	0.42
1:L:199:THR:HG22	1:L:204:THR:OG1	2.20	0.42
2:H:151:THR:O	2:H:197:VAL:HA	2.20	0.42
2:H:151:THR:HG22	5:H:337:HOH:O	2.20	0.42
1:L:156:THR:HA	1:L:157:PRO:HD3	1.82	0.41
1:L:52:GLY:O	1:L:54:ASN:ND2	2.54	0.41
1:L:5:THR:CG2	1:L:23:ARG:HB3	2.48	0.40
1:L:139:ILE:CG2	1:L:198:VAL:HG11	2.51	0.40
1:L:6:GLN:HB3	5:L:336:HOH:O	2.22	0.40
2:H:138:LEU:CD1	2:H:188:ARG:HG3	2.49	0.40
1:L:12:THR:HG21	1:L:18:VAL:HB	2.03	0.40
1:L:188:TRP:CZ2	1:L:211:ARG:HG3	2.56	0.40
1:L:88:TYR:O	1:L:103:GLY:HA2	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	L	209/215 (97%)	197 (94%)	10 (5%)	2 (1%)	13 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	211/226 (93%)	191 (90%)	20 (10%)	0	100	100
All	All	420/441 (95%)	388 (92%)	30 (7%)	2 (0%)	25	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	96	ASN
1	L	54	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	179/182 (98%)	156 (87%)	23 (13%)	3	3
2	H	182/194 (94%)	152 (84%)	30 (16%)	2	1
All	All	361/376 (96%)	308 (85%)	53 (15%)	2	2

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	12	THR
1	L	38	VAL
1	L	44	HIS
1	L	54	ASN
1	L	65	SER
1	L	69	ILE
1	L	71	ASP
1	L	81	GLN
1	L	96	ASN
1	L	113	LYS
1	L	120	LEU
1	L	132	LYS
1	L	140	ILE
1	L	147	VAL

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Mol	Chain	Res	Type
1	L	160	GLN
1	L	166	GLN
1	L	168	SER
1	L	169	LYS
1	L	186	ARG
1	L	187	GLU
1	L	193	SER
1	L	201	GLU
1	L	207	LYS
2	H	3	THR
2	H	5	VAL
2	H	6	GLU
2	H	7	SER
2	H	19	LYS
2	H	38	ARG
2	H	43	LYS
2	H	44	ARG
2	H	58	THR
2	H	61	SER
2	H	63	SER
2	H	68	PHE
2	H	77	ASN
2	H	78	ASN
2	H	83	LEU
2	H	87	ARG
2	H	106	HIS
2	H	115	LYS
2	H	134	SER
2	H	140	CYS
2	H	148	GLU
2	H	156	SER
2	H	170	LEU
2	H	171	GLU
2	H	178	SER
2	H	188	ARG
2	H	192	THR
2	H	203	SER
2	H	212	PRO
2	H	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	33	ASN
1	L	39	GLN
1	L	54	ASN
1	L	81	GLN
1	L	160	GLN
1	L	170	GLN
2	H	39	GLN
2	H	77	ASN
2	H	78	ASN
2	H	131	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)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
4	EOT	H	801	3	34,34,34	1.77	9 (26%)	42,44,44	1.24	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EOT	H	801	3	-	7/36/36/36	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	801	EOT	O5-C8	4.08	1.35	1.22
4	H	801	EOT	O1-C4	4.08	1.35	1.22
4	H	801	EOT	O7-C10	4.01	1.35	1.22
4	H	801	EOT	O3-C6	3.84	1.34	1.22
4	H	801	EOT	C15-N3	-3.58	1.34	1.41
4	H	801	EOT	O8-C10	-2.33	1.23	1.30
4	H	801	EOT	O6-C8	-2.24	1.23	1.30
4	H	801	EOT	O4-C6	-2.20	1.23	1.30
4	H	801	EOT	O2-C4	-2.16	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	801	EOT	O2-C4-C3	2.25	122.27	113.38
4	H	801	EOT	C5-N2-C2	-2.09	107.59	111.95
4	H	801	EOT	O4-C6-C5	2.02	121.36	113.38
4	H	801	EOT	O8-C10-C9	2.01	121.30	113.38
4	H	801	EOT	O6-C8-C7	2.01	121.30	113.38

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	801	EOT	O8-C10-C9-N1
4	H	801	EOT	C20-C19-N4-C18
4	H	801	EOT	C6-C5-N2-C2
4	H	801	EOT	C6-C5-N2-C3
4	H	801	EOT	N1-C7-C8-O6
4	H	801	EOT	O7-C10-C9-N1
4	H	801	EOT	C11-C1-C2-N2

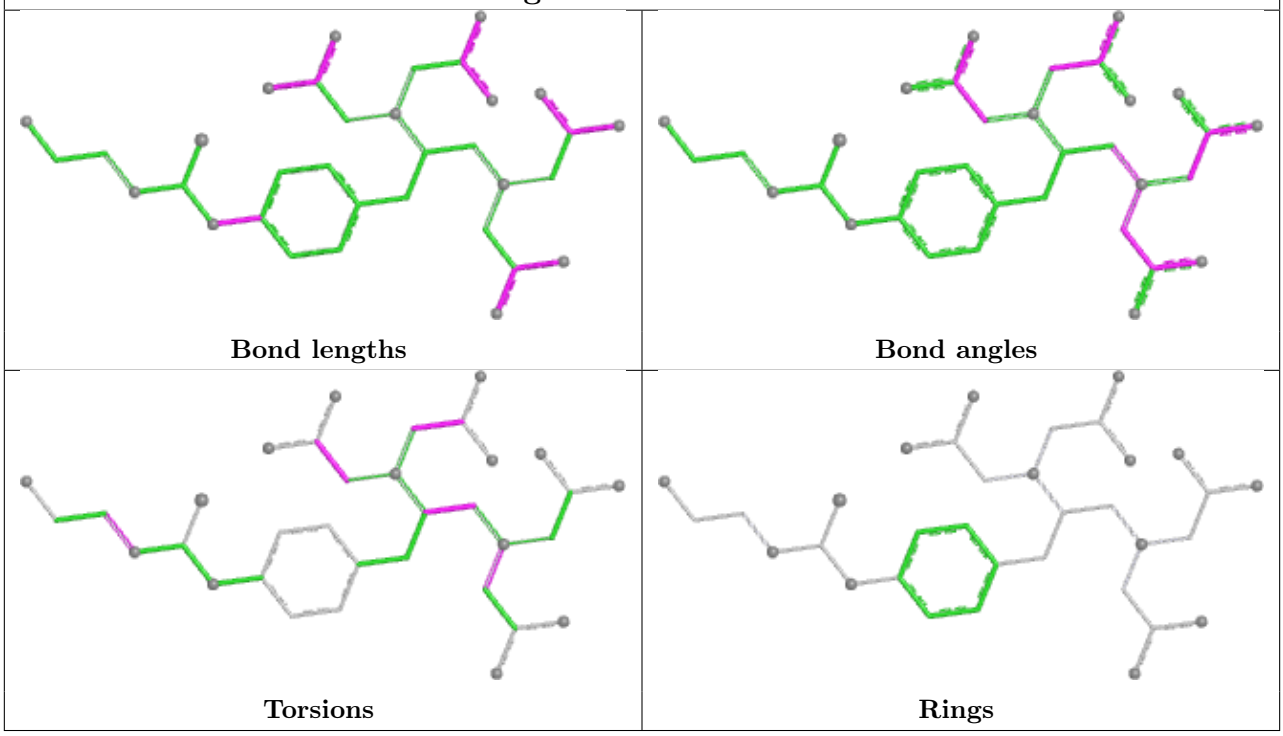
There are no ring outliers.

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 EOT H 801



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.