



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:15 AM UTC

PDB ID : 1INE / pdb_00001ine
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 : 2.80 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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

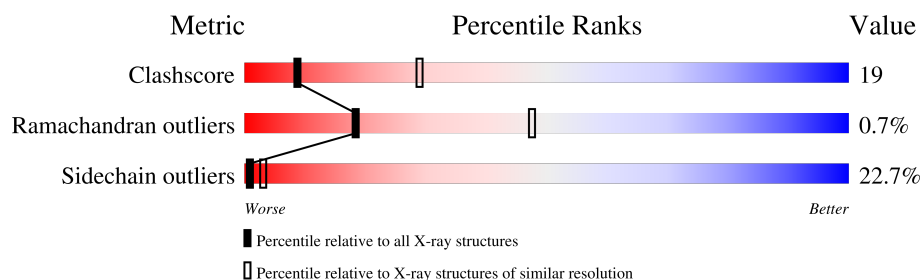
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	215	
2	H	226	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3371 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
1	L	211	Total	C	N	O	S	0	0	0
			1601	1002	270	323	6			

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
2	H	213	Total	C	N	O	S	0	0	0
			1593	1004	271	312	6			

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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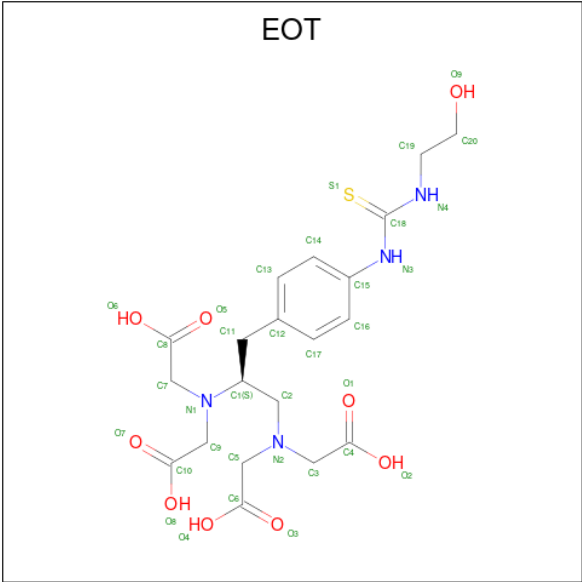
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Chain	Residue	Modelled	Actual	Comment	Reference
H	56	GLY	THR	conflict	PIR S38864
H	57	PHE	TYR	conflict	PIR S38864
H	59	PHE	TYR	conflict	PIR S38864
H	61	SER	PRO	conflict	PIR S38864
H	62	ALA	ASP	conflict	PIR S38864
H	76	GLN	LYS	conflict	PIR S38864
H	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 FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Fe 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 (CCD ID: EOT) (formula: C₂₀H₂₈N₄O₉S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	67	Total	O	0	0
			67	67		
5	H	75	Total	O	0	0
			75	75		

3 Residue-property plots [i](#)

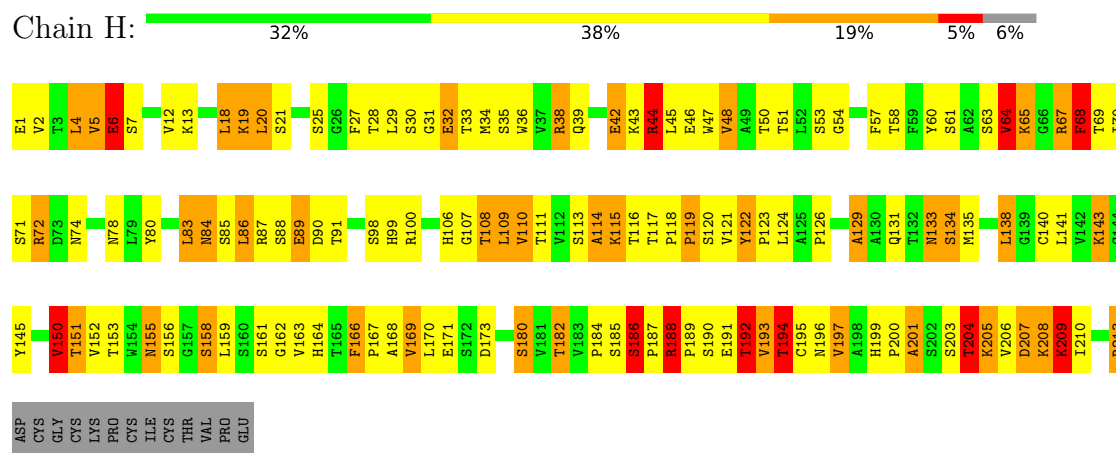
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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)



• Molecule 2: IGG1-LAMBDA CHA255 FAB (HEAVY CHAIN)



4 Data and refinement statistics

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	99.90Å 85.60Å 77.50Å 90.00° 136.40° 90.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, TNT, X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3371	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: FE, 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	1.34	5/1638 (0.3%)	2.29	80/2238 (3.6%)
2	H	1.39	8/1633 (0.5%)	2.54	141/2231 (6.3%)
All	All	1.36	13/3271 (0.4%)	2.42	221/4469 (4.9%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	71	ASP	N-CA	7.12	1.54	1.46
2	H	115	LYS	N-CA	6.84	1.55	1.46
1	L	41	LYS	N-CA	6.26	1.53	1.45
2	H	110	VAL	CA-C	6.09	1.59	1.52
1	L	78	THR	CA-CB	5.92	1.60	1.53
2	H	116	THR	N-CA	5.89	1.53	1.46
1	L	62	ALA	C-N	-5.67	1.26	1.33
2	H	115	LYS	CA-C	5.62	1.59	1.52
2	H	114	ALA	C-N	5.54	1.40	1.33
2	H	98	SER	C-N	-5.37	1.26	1.33
1	L	98	TRP	NE1-CE2	-5.36	1.31	1.37
2	H	85	SER	N-CA	5.03	1.53	1.46
2	H	90	ASP	C-O	5.03	1.30	1.24

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	L	187	GLU	CB-CG-CD	12.38	133.65	112.60
2	H	155	ASN	CA-CB-CG	11.67	124.27	112.60
2	H	32	GLU	CB-CG-CD	11.21	131.65	112.60
2	H	57	PHE	CA-CB-CG	10.88	124.68	113.80
1	L	44	HIS	CA-CB-CG	10.86	124.66	113.80
2	H	6	GLU	CA-CB-CG	10.36	134.83	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	158	VAL	CB-CA-C	10.12	124.93	111.88
2	H	213	ARG	N-CA-C	9.59	137.86	111.00
1	L	126	GLU	CA-CB-CG	9.30	132.70	114.10
2	H	68	PHE	CA-CB-CG	9.23	123.03	113.80
2	H	134	SER	CA-C-N	9.09	136.74	122.74
2	H	134	SER	C-N-CA	9.09	136.74	122.74
1	L	99	VAL	N-CA-CB	8.94	123.26	111.64
1	L	126	GLU	CB-CG-CD	8.76	127.48	112.60
2	H	64	VAL	N-CA-CB	-8.71	96.85	111.23
2	H	108	THR	CA-C-O	8.57	130.01	119.98
1	L	55	ASN	O-C-N	8.29	133.21	123.02
1	L	41	LYS	CB-CA-C	8.28	121.57	109.48
2	H	129	ALA	CA-C-N	8.28	140.17	123.20
2	H	129	ALA	C-N-CA	8.28	140.17	123.20
2	H	54	GLY	N-CA-C	-8.26	93.60	113.18
2	H	99	HIS	CA-CB-CG	8.24	122.05	113.80
1	L	71	ASP	CA-CB-CG	8.20	120.80	112.60
2	H	84	ASN	CA-C-N	-8.14	110.02	123.37
2	H	84	ASN	C-N-CA	-8.14	110.02	123.37
1	L	43	ASP	CA-CB-CG	8.12	120.72	112.60
1	L	23	ARG	CD-NE-CZ	8.08	135.71	124.40
1	L	122	PRO	CA-C-N	8.07	128.00	119.85
1	L	122	PRO	C-N-CA	8.07	128.00	119.85
1	L	71	ASP	CB-CA-C	8.01	123.43	111.17
2	H	28	THR	CA-C-N	7.96	130.94	120.28
2	H	28	THR	C-N-CA	7.96	130.94	120.28
1	L	150	ASP	CA-CB-CG	7.93	120.53	112.60
2	H	159	LEU	CB-CA-C	7.87	123.36	110.22
1	L	71	ASP	N-CA-CB	-7.76	99.63	110.65
2	H	84	ASN	N-CA-C	7.71	122.59	112.72
1	L	139	ILE	CB-CA-C	7.68	122.00	110.63
2	H	110	VAL	N-CA-CB	7.58	124.58	111.39
1	L	69	ILE	CB-CA-C	7.50	120.32	110.12
2	H	86	LEU	CB-CA-C	7.50	121.88	109.89
2	H	151	THR	CB-CA-C	7.46	122.07	110.14
1	L	160	GLN	N-CA-C	7.45	120.54	108.76
2	H	106	HIS	N-CA-C	7.45	121.81	112.87
2	H	169	VAL	CB-CA-C	7.42	120.21	110.12
2	H	129	ALA	N-CA-C	7.36	119.47	110.41
2	H	122	TYR	CB-CA-C	7.33	119.90	110.16
2	H	145	TYR	CA-CB-CG	7.25	126.94	113.90
2	H	5	VAL	CB-CA-C	7.17	120.11	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	142	PHE	CA-CB-CG	7.17	120.97	113.80
2	H	85	SER	O-C-N	7.11	132.06	122.82
2	H	169	VAL	CA-CB-CG1	7.11	122.48	110.40
2	H	1	GLU	CB-CG-CD	7.07	124.62	112.60
2	H	110	VAL	N-CA-C	-7.04	98.35	108.48
1	L	158	VAL	CA-C-O	7.02	129.25	121.04
2	H	20	LEU	O-C-N	-7.01	115.11	123.03
1	L	147	VAL	O-C-N	7.01	129.07	122.97
2	H	29	LEU	CA-C-N	6.99	129.98	120.54
2	H	29	LEU	C-N-CA	6.99	129.98	120.54
2	H	155	ASN	OD1-CG-ND2	-6.98	115.62	122.60
2	H	46	GLU	CA-CB-CG	6.90	127.91	114.10
2	H	158	SER	CA-C-N	-6.82	113.09	122.30
2	H	158	SER	C-N-CA	-6.82	113.09	122.30
2	H	186	SER	CB-CA-C	6.79	123.55	110.17
1	L	172	ASN	CA-CB-CG	6.77	119.37	112.60
2	H	48	VAL	O-C-N	6.76	126.98	121.85
2	H	29	LEU	N-CA-C	6.71	118.59	111.28
1	L	140	ILE	CA-CB-CG2	6.61	121.73	110.50
2	H	87	ARG	CD-NE-CZ	6.60	133.64	124.40
2	H	170	LEU	CA-C-O	-6.58	113.10	120.54
2	H	89	GLU	CA-CB-CG	6.58	127.25	114.10
2	H	64	VAL	CA-CB-CG1	6.55	121.53	110.40
1	L	34	TYR	CA-CB-CG	6.51	125.62	113.90
2	H	36	TRP	N-CA-CB	6.46	120.72	110.65
2	H	63	SER	CA-C-N	6.45	133.58	121.97
2	H	63	SER	C-N-CA	6.45	133.58	121.97
1	L	29	VAL	N-CA-C	-6.39	101.31	109.80
1	L	85	GLU	N-CA-C	-6.37	99.98	109.15
2	H	108	THR	N-CA-CB	6.35	119.64	110.37
2	H	117	THR	CA-C-N	6.27	126.84	120.38
2	H	117	THR	C-N-CA	6.27	126.84	120.38
1	L	166	GLN	CB-CG-CD	6.27	123.25	112.60
1	L	208	SER	CA-C-O	6.27	128.36	121.40
2	H	119	PRO	O-C-N	6.26	130.77	123.06
2	H	45	LEU	O-C-N	6.25	130.33	123.27
1	L	81	GLN	CB-CG-CD	6.24	123.20	112.60
1	L	201	GLU	CA-CB-CG	6.22	126.55	114.10
1	L	108	VAL	N-CA-C	-6.21	96.84	106.72
2	H	168	ALA	CA-C-N	6.19	132.17	122.70
2	H	168	ALA	C-N-CA	6.19	132.17	122.70
2	H	47	TRP	CA-C-N	-6.18	116.92	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	47	TRP	C-N-CA	-6.18	116.92	122.97
1	L	195	SER	CA-C-N	6.13	131.65	123.00
1	L	195	SER	C-N-CA	6.13	131.65	123.00
2	H	194	THR	CA-CB-CG2	6.11	120.89	110.50
2	H	54	GLY	O-C-N	6.10	130.63	122.70
2	H	90	ASP	N-CA-C	6.10	120.45	112.89
2	H	50	THR	O-C-N	6.09	130.79	123.36
1	L	47	THR	CA-C-N	6.06	126.85	120.43
1	L	47	THR	C-N-CA	6.06	126.85	120.43
2	H	83	LEU	CA-CB-CG	6.04	137.43	116.30
2	H	122	TYR	CA-C-O	6.04	125.21	119.72
1	L	45	LEU	CB-CA-C	6.02	120.14	109.72
1	L	205	VAL	N-CA-C	-6.01	99.47	108.12
1	L	10	LEU	CA-C-O	5.99	128.22	121.51
1	L	196	CYS	N-CA-CB	5.99	119.99	110.65
1	L	160	GLN	CB-CG-CD	5.98	122.77	112.60
2	H	182	THR	O-C-N	5.97	130.26	123.27
2	H	118	PRO	CA-C-N	5.97	125.88	119.85
2	H	118	PRO	C-N-CA	5.97	125.88	119.85
2	H	210	ILE	CA-C-N	5.97	133.17	122.13
2	H	210	ILE	C-N-CA	5.97	133.17	122.13
1	L	33	ASN	CA-C-N	5.96	130.86	122.46
1	L	33	ASN	C-N-CA	5.96	130.86	122.46
2	H	193	VAL	CB-CA-C	5.94	119.20	110.77
1	L	77	ILE	CA-C-N	5.92	130.81	121.99
1	L	77	ILE	C-N-CA	5.92	130.81	121.99
2	H	173	ASP	CA-CB-CG	5.89	118.49	112.60
1	L	204	THR	N-CA-CB	5.84	118.88	110.06
1	L	88	TYR	N-CA-C	5.83	118.31	107.99
2	H	192	THR	CA-C-N	5.82	130.84	123.10
2	H	192	THR	C-N-CA	5.82	130.84	123.10
1	L	70	GLY	N-CA-C	-5.82	101.67	112.37
2	H	188	ARG	CB-CG-CD	5.81	124.66	111.30
1	L	198	VAL	CB-CA-C	5.78	118.51	110.99
2	H	42	GLU	CA-CB-CG	5.78	125.66	114.10
1	L	161	GLY	CA-C-O	5.78	126.64	119.88
2	H	199	HIS	N-CA-C	-5.76	97.08	109.81
2	H	69	THR	CA-C-N	5.74	130.72	122.45
2	H	69	THR	C-N-CA	5.74	130.72	122.45
2	H	143	LYS	CA-C-N	5.74	132.66	121.41
2	H	143	LYS	C-N-CA	5.74	132.66	121.41
1	L	197	GLN	CA-CB-CG	5.73	125.57	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	190	ARG	CD-NE-CZ	5.70	132.38	124.40
1	L	169	LYS	CA-CB-CG	5.64	125.38	114.10
2	H	7	SER	CA-C-N	-5.61	116.77	123.44
2	H	7	SER	C-N-CA	-5.61	116.77	123.44
2	H	210	ILE	CB-CA-C	5.60	117.28	111.23
1	L	184	THR	N-CA-C	-5.59	102.63	110.35
2	H	204	THR	CA-C-O	5.59	126.47	120.38
2	H	205	LYS	N-CA-C	-5.58	99.34	108.76
2	H	42	GLU	CA-C-N	5.57	130.76	122.74
2	H	42	GLU	C-N-CA	5.57	130.76	122.74
1	L	135	LEU	N-CA-C	-5.56	100.65	109.76
2	H	6	GLU	CB-CG-CD	5.55	122.04	112.60
2	H	193	VAL	CA-C-O	5.55	126.16	120.39
2	H	186	SER	CA-C-N	5.55	125.65	119.32
2	H	186	SER	C-N-CA	5.55	125.65	119.32
1	L	30	THR	CA-C-N	5.54	128.26	120.28
1	L	30	THR	C-N-CA	5.54	128.26	120.28
2	H	44	ARG	CD-NE-CZ	5.53	132.14	124.40
2	H	150	VAL	CA-CB-CG1	5.53	119.80	110.40
2	H	162	GLY	CA-C-N	5.53	128.50	120.98
2	H	162	GLY	C-N-CA	5.53	128.50	120.98
1	L	175	TYR	CA-CB-CG	5.52	123.84	113.90
1	L	103	GLY	CA-C-N	5.51	130.54	122.77
1	L	103	GLY	C-N-CA	5.51	130.54	122.77
2	H	195	CYS	CA-C-N	5.50	130.50	122.85
2	H	195	CYS	C-N-CA	5.50	130.50	122.85
2	H	110	VAL	CA-CB-CG2	5.49	119.73	110.40
2	H	204	THR	CA-CB-CG2	5.49	119.83	110.50
2	H	106	HIS	CA-CB-CG	5.46	119.26	113.80
2	H	72	ARG	NE-CZ-NH1	5.45	126.95	121.50
2	H	166	PHE	CA-C-N	5.45	125.39	119.78
2	H	166	PHE	C-N-CA	5.45	125.39	119.78
2	H	155	ASN	CA-C-O	5.42	128.26	120.51
2	H	120	SER	CA-C-O	5.38	126.12	120.36
2	H	100	ARG	CA-C-N	5.36	131.78	121.54
2	H	100	ARG	C-N-CA	5.36	131.78	121.54
2	H	192	THR	O-C-N	5.36	129.26	123.10
2	H	5	VAL	CA-CB-CG1	5.35	119.49	110.40
2	H	150	VAL	CA-C-N	-5.35	115.23	122.77
2	H	150	VAL	C-N-CA	-5.35	115.23	122.77
1	L	104	THR	CA-CB-CG2	5.33	119.56	110.50
2	H	46	GLU	CB-CG-CD	5.32	121.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	5	VAL	O-C-N	5.32	128.71	123.18
1	L	47	THR	CA-CB-CG2	5.32	119.54	110.50
1	L	63	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	L	160	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	L	157	PRO	CA-C-N	-5.28	115.89	122.48
1	L	157	PRO	C-N-CA	-5.28	115.89	122.48
1	L	5	THR	CA-CB-CG2	5.27	119.46	110.50
1	L	21	THR	CA-C-N	5.27	131.19	122.33
1	L	21	THR	C-N-CA	5.27	131.19	122.33
2	H	159	LEU	N-CA-C	-5.27	100.58	108.96
2	H	88	SER	CB-CA-C	-5.26	102.39	110.81
2	H	85	SER	CB-CA-C	5.25	119.48	111.76
1	L	69	ILE	CA-CB-CG2	5.25	119.42	110.50
2	H	87	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	L	105	LYS	CA-CB-CG	5.24	124.58	114.10
1	L	21	THR	CB-CA-C	5.22	120.06	110.24
2	H	208	LYS	CA-C-N	-5.21	115.84	122.77
2	H	208	LYS	C-N-CA	-5.21	115.84	122.77
1	L	135	LEU	CA-CB-CG	5.20	134.50	116.30
2	H	155	ASN	CA-C-N	5.18	131.44	121.54
2	H	155	ASN	C-N-CA	5.18	131.44	121.54
2	H	110	VAL	O-C-N	5.18	128.78	123.18
2	H	209	LYS	N-CA-CB	5.16	118.83	110.42
1	L	170	GLN	OE1-CD-NE2	-5.16	117.44	122.60
2	H	201	ALA	CA-C-O	-5.16	114.98	121.02
1	L	185	ALA	CA-C-N	5.14	129.37	120.58
1	L	185	ALA	C-N-CA	5.14	129.37	120.58
1	L	46	PHE	CA-CB-CG	5.14	118.94	113.80
2	H	109	LEU	N-CA-CB	-5.14	102.20	109.85
2	H	188	ARG	CD-NE-CZ	5.12	131.57	124.40
2	H	213	ARG	N-CA-CB	-5.11	101.81	110.50
2	H	4	LEU	CA-C-N	-5.11	115.73	122.98
2	H	4	LEU	C-N-CA	-5.11	115.73	122.98
2	H	191	GLU	CB-CG-CD	5.11	121.28	112.60
1	L	23	ARG	CB-CG-CD	5.10	123.02	111.30
2	H	134	SER	CA-CB-OG	5.08	121.27	111.10
2	H	67	ARG	CD-NE-CZ	5.08	131.51	124.40
2	H	207	ASP	CA-CB-CG	5.07	117.67	112.60
1	L	209	LEU	O-C-N	5.06	129.33	123.41
2	H	85	SER	N-CA-C	-5.04	98.14	107.71
2	H	115	LYS	N-CA-C	5.03	116.08	108.07
2	H	206	VAL	CA-CB-CG1	5.03	118.95	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	33	THR	CA-CB-CG2	5.02	119.04	110.50
1	L	11	THR	CA-CB-CG2	5.01	119.02	110.50
2	H	33	THR	N-CA-C	-5.01	101.14	109.46
2	H	38	ARG	CB-CG-CD	5.01	122.83	111.30
2	H	208	LYS	O-C-N	5.01	129.17	123.31

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	L	1601	0	1550	65	0
2	H	1593	0	1570	57	0
3	H	1	0	0	0	0
4	H	34	0	24	0	0
5	H	75	0	0	17	0
5	L	67	0	0	10	0
All	All	3371	0	3144	119	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 19.

All (119) 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:82:THR:HG23	5:L:370:HOH:O	1.57	1.05
1:L:164:THR:HG22	5:L:395:HOH:O	1.58	1.02
2:H:190:SER:HB2	5:H:430:HOH:O	1.60	0.99
1:L:30:THR:H	1:L:33:ASN:HD22	1.14	0.93
1:L:138:THR:HG21	5:H:392:HOH:O	1.69	0.93
1:L:205:VAL:HG13	5:L:409:HOH:O	1.69	0.92
2:H:91:THR:HG23	2:H:111:THR:HA	1.52	0.91
1:L:5:THR:HB	5:L:340:HOH:O	1.73	0.86
2:H:138:LEU:HD11	2:H:188:ARG:HG3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:188:ARG:HD2	2:H:189:PRO:HA	1.66	0.77
1:L:23:ARG:HB2	1:L:72:LYS:HG2	1.66	0.77
2:H:121:VAL:HG21	2:H:197:VAL:HG11	1.68	0.76
1:L:164:THR:CG2	5:L:395:HOH:O	2.22	0.76
2:H:48:VAL:HG13	2:H:64:VAL:HG21	1.66	0.75
2:H:126:PRO:HB2	2:H:129:ALA:HB2	1.71	0.72
1:L:30:THR:H	1:L:33:ASN:ND2	1.87	0.71
2:H:151:THR:O	5:H:336:HOH:O	2.08	0.70
1:L:140:ILE:HD11	2:H:166:PHE:HZ	1.57	0.70
1:L:39:GLN:NE2	1:L:41:LYS:HG3	2.08	0.68
1:L:141:ASP:H	1:L:170:GLN:HE22	1.41	0.68
2:H:192:THR:HG21	5:H:322:HOH:O	1.94	0.67
1:L:23:ARG:NH2	5:L:305:HOH:O	2.27	0.67
1:L:162:MET:HA	1:L:180:TYR:O	1.96	0.66
1:L:38:VAL:HG12	1:L:48:GLY:HA2	1.78	0.66
1:L:164:THR:HG23	1:L:179:SER:HB2	1.78	0.65
1:L:138:THR:CG2	5:H:392:HOH:O	2.38	0.64
1:L:147:VAL:HG21	1:L:198:VAL:HG13	1.81	0.63
2:H:209:LYS:HD2	5:H:322:HOH:O	1.97	0.63
1:L:54:ASN:ND2	1:L:55:ASN:OD1	2.33	0.61
1:L:139:ILE:HG12	1:L:198:VAL:HG21	1.83	0.60
2:H:109:LEU:HD11	5:H:360:HOH:O	2.02	0.58
1:L:53:THR:HG22	1:L:53:THR:O	2.03	0.58
2:H:133:ASN:OD1	5:H:339:HOH:O	2.17	0.58
1:L:12:THR:HG21	1:L:18:VAL:HB	1.87	0.57
1:L:63:ARG:HH21	1:L:81:GLN:HG2	1.69	0.57
1:L:68:LEU:HD23	1:L:73:ALA:HA	1.85	0.57
2:H:32:GLU:HG3	2:H:34:MET:HE2	1.85	0.56
1:L:153:VAL:HG22	1:L:194:TYR:CD1	2.40	0.56
2:H:151:THR:C	5:H:336:HOH:O	2.49	0.55
1:L:78:THR:HG22	5:L:379:HOH:O	2.06	0.55
1:L:153:VAL:HG22	1:L:194:TYR:HD1	1.71	0.55
1:L:172:ASN:OD1	1:L:174:LYS:HB2	2.06	0.55
2:H:184:PRO:O	2:H:187:PRO:HD2	2.06	0.55
1:L:140:ILE:HG12	2:H:164:HIS:CD2	2.42	0.55
2:H:31:GLY:HA2	2:H:53:SER:HB2	1.88	0.55
1:L:147:VAL:CG2	1:L:198:VAL:HG13	2.37	0.55
1:L:33:ASN:HA	1:L:93:TRP:O	2.07	0.54
2:H:126:PRO:HB2	2:H:129:ALA:CB	2.37	0.54
2:H:121:VAL:CG2	2:H:197:VAL:HG11	2.38	0.53
2:H:163:VAL:HA	2:H:180:SER:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:121:VAL:HG21	2:H:197:VAL:CG1	2.38	0.53
1:L:63:ARG:O	1:L:63:ARG:HG2	2.08	0.52
1:L:191:HIS:O	1:L:211:ARG:HD3	2.09	0.52
1:L:85:GLU:HG3	1:L:106:LEU:O	2.10	0.52
1:L:105:LYS:HD3	5:L:328:HOH:O	2.11	0.51
1:L:149:VAL:HG22	1:L:198:VAL:HG22	1.92	0.51
1:L:15:GLY:O	1:L:79:GLY:HA2	2.11	0.51
2:H:133:ASN:HB3	5:H:339:HOH:O	2.11	0.51
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.92	0.51
2:H:67:ARG:O	2:H:84:ASN:HB2	2.11	0.51
2:H:185:SER:HB2	5:H:433:HOH:O	2.11	0.51
1:L:5:THR:HG22	1:L:23:ARG:HG2	1.93	0.51
2:H:143:LYS:HE3	5:H:377:HOH:O	2.09	0.51
1:L:39:GLN:HE21	1:L:41:LYS:HG3	1.76	0.50
2:H:6:GLU:HA	2:H:21:SER:O	2.11	0.50
2:H:113:SER:OG	2:H:114:ALA:N	2.45	0.50
2:H:83:LEU:HD12	2:H:86:LEU:HD21	1.92	0.50
1:L:64:PHE:CE2	1:L:77:ILE:HG12	2.47	0.50
1:L:158:VAL:HG11	1:L:181:LEU:HD21	1.93	0.50
2:H:213:ARG:HB2	5:H:414:HOH:O	2.11	0.49
1:L:208:SER:HB2	5:L:434:HOH:O	2.12	0.49
1:L:82:THR:CG2	5:L:370:HOH:O	2.35	0.49
1:L:39:GLN:NE2	1:L:41:LYS:HE2	2.28	0.48
2:H:131:GLN:HB2	2:H:134:SER:HA	1.96	0.48
1:L:40:GLU:HB2	1:L:46:PHE:CE2	2.49	0.48
2:H:194:THR:HG22	2:H:196:ASN:HD21	1.79	0.48
2:H:6:GLU:CD	2:H:107:GLY:H	2.22	0.48
2:H:158:SER:HB3	5:H:425:HOH:O	2.13	0.47
1:L:39:GLN:HB2	1:L:49:LEU:HD11	1.95	0.47
1:L:39:GLN:HE22	1:L:41:LYS:HE2	1.79	0.47
2:H:78:ASN:HB3	2:H:80:TYR:CE1	2.50	0.47
2:H:39:GLN:HA	2:H:44:ARG:O	2.15	0.47
1:L:206:GLU:O	1:L:207:LYS:NZ	2.48	0.47
2:H:135:MET:HG3	2:H:182:THR:HG22	1.96	0.47
2:H:64:VAL:HG22	2:H:68:PHE:CE2	2.50	0.46
2:H:151:THR:HG22	5:H:336:HOH:O	2.14	0.46
2:H:74:ASN:HA	5:H:333:HOH:O	2.15	0.46
2:H:186:SER:OG	2:H:187:PRO:HD3	2.16	0.46
1:L:167:PRO:HA	1:L:176:MET:O	2.17	0.45
1:L:192:SER:HA	1:L:211:ARG:HB3	1.97	0.45
1:L:168:SER:O	1:L:175:TYR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:123:PRO:HG3	2:H:208:LYS:HD2	2.00	0.44
1:L:23:ARG:HD2	1:L:72:LYS:HE3	1.98	0.44
1:L:64:PHE:CD2	1:L:77:ILE:HG12	2.53	0.44
2:H:2:VAL:HG13	2:H:27:PHE:CE1	2.52	0.44
1:L:54:ASN:HD22	1:L:55:ASN:CG	2.26	0.44
2:H:190:SER:CB	5:H:430:HOH:O	2.36	0.44
1:L:35:ALA:HA	1:L:92:LEU:HD23	1.98	0.43
2:H:119:PRO:HD2	2:H:204:THR:HG21	2.00	0.43
2:H:18:LEU:O	2:H:83:LEU:N	2.50	0.43
2:H:60:TYR:HB2	2:H:65:LYS:HD2	2.00	0.43
2:H:122:TYR:HA	2:H:123:PRO:HD3	1.71	0.43
2:H:200:PRO:O	2:H:201:ALA:C	2.61	0.43
1:L:140:ILE:HG23	1:L:141:ASP:OD2	2.19	0.43
1:L:7:GLU:O	1:L:104:THR:OG1	2.35	0.42
1:L:166:GLN:HE22	2:H:167:PRO:HG3	1.83	0.42
1:L:22:CYS:HB3	1:L:73:ALA:HB3	2.00	0.42
1:L:120:LEU:HD13	1:L:209:LEU:HD21	2.01	0.42
2:H:124:LEU:HD11	2:H:141:LEU:HB2	2.01	0.42
1:L:94:TYR:CD2	1:L:99:VAL:HG23	2.54	0.42
1:L:156:THR:HA	1:L:157:PRO:HD3	1.86	0.42
2:H:155:ASN:OD1	2:H:193:VAL:HA	2.20	0.41
1:L:120:LEU:HD13	1:L:209:LEU:CD2	2.50	0.41
1:L:139:ILE:HG22	1:L:142:PHE:CD2	2.55	0.41
2:H:19:LYS:HD2	2:H:80:TYR:HB3	2.01	0.41
2:H:51:THR:HG23	2:H:72:ARG:NH2	2.36	0.41
1:L:94:TYR:HD2	1:L:99:VAL:HG23	1.86	0.40
2:H:150:VAL:HG13	2:H:152:VAL:HG23	2.02	0.40
2:H:188:ARG:HB3	2:H:188:ARG:HH11	1.86	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%)	189 (90%)	17 (8%)	3 (1%)	9	30
2	H	211/226 (93%)	187 (89%)	24 (11%)	0	100	100
All	All	420/441 (95%)	376 (90%)	41 (10%)	3 (1%)	18	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	96	ASN
1	L	54	ASN
1	L	109	LEU

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	L	179/182 (98%)	142 (79%)	37 (21%)	1	4
2	H	182/194 (94%)	137 (75%)	45 (25%)	1	2
All	All	361/376 (96%)	279 (77%)	82 (23%)	1	3

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	11	THR
1	L	44	HIS
1	L	45	LEU
1	L	47	THR
1	L	50	ILE
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	111	GLN

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Mol	Chain	Res	Type
1	L	113	LYS
1	L	119	THR
1	L	120	LEU
1	L	124	SER
1	L	127	GLU
1	L	132	LYS
1	L	135	LEU
1	L	140	ILE
1	L	146	VAL
1	L	158	VAL
1	L	160	GLN
1	L	162	MET
1	L	164	THR
1	L	166	GLN
1	L	168	SER
1	L	169	LYS
1	L	183	LEU
1	L	186	ARG
1	L	193	SER
1	L	199	THR
1	L	207	LYS
1	L	209	LEU
1	L	210	SER
1	L	211	ARG
2	H	4	LEU
2	H	5	VAL
2	H	6	GLU
2	H	13	LYS
2	H	18	LEU
2	H	19	LYS
2	H	20	LEU
2	H	25	SER
2	H	30	SER
2	H	35	SER
2	H	38	ARG
2	H	42	GLU
2	H	43	LYS
2	H	44	ARG
2	H	58	THR
2	H	61	SER
2	H	64	VAL
2	H	65	LYS

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Mol	Chain	Res	Type
2	H	68	PHE
2	H	70	ILE
2	H	71	SER
2	H	89	GLU
2	H	108	THR
2	H	110	VAL
2	H	115	LYS
2	H	133	ASN
2	H	138	LEU
2	H	140	CYS
2	H	150	VAL
2	H	153	THR
2	H	156	SER
2	H	161	SER
2	H	169	VAL
2	H	171	GLU
2	H	180	SER
2	H	186	SER
2	H	188	ARG
2	H	192	THR
2	H	194	THR
2	H	197	VAL
2	H	203	SER
2	H	204	THR
2	H	205	LYS
2	H	207	ASP
2	H	209	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	33	ASN
1	L	39	GLN
1	L	44	HIS
1	L	54	ASN
1	L	111	GLN
1	L	166	GLN
1	L	170	GLN
1	L	197	GLN
2	H	74	ASN
2	H	77	ASN
2	H	103	HIS

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Mol	Chain	Res	Type
2	H	133	ASN
2	H	164	HIS
2	H	196	ASN

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	1.82	12 (35%)	42,44,44	1.41	9 (21%)

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	-	3/36/36/36	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	801	EOT	C7-N1	3.59	1.56	1.47
4	H	801	EOT	C11-C1	3.26	1.58	1.53
4	H	801	EOT	O5-C8	3.25	1.32	1.22
4	H	801	EOT	C11-C12	-2.90	1.44	1.51
4	H	801	EOT	O6-C8	-2.86	1.21	1.30
4	H	801	EOT	O2-C4	-2.73	1.21	1.30
4	H	801	EOT	C7-C8	-2.43	1.46	1.51
4	H	801	EOT	O8-C10	-2.42	1.22	1.30
4	H	801	EOT	O1-C4	2.36	1.29	1.22
4	H	801	EOT	C15-N3	-2.28	1.37	1.41
4	H	801	EOT	O7-C10	2.24	1.29	1.22
4	H	801	EOT	O3-C6	2.19	1.29	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	801	EOT	C12-C11-C1	-2.72	107.96	113.22
4	H	801	EOT	C11-C12-C13	-2.67	115.93	120.90
4	H	801	EOT	O2-C4-C3	2.62	123.69	113.38
4	H	801	EOT	O6-C8-C7	2.30	122.43	113.38
4	H	801	EOT	O1-C4-C3	-2.25	112.99	122.38
4	H	801	EOT	C15-N3-C18	2.22	134.71	128.54
4	H	801	EOT	O4-C6-C5	2.18	121.97	113.38
4	H	801	EOT	C20-C19-N4	-2.17	106.48	111.60
4	H	801	EOT	O8-C10-C9	2.11	121.69	113.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

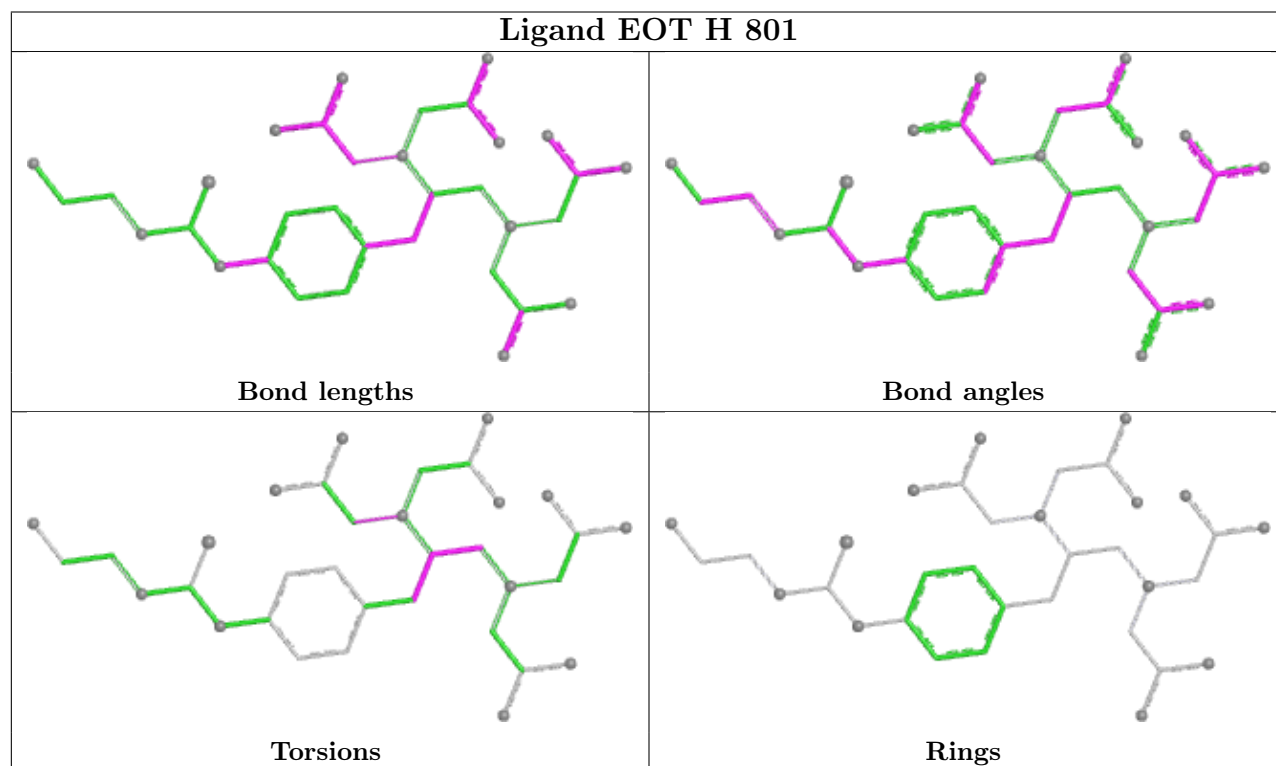
Mol	Chain	Res	Type	Atoms
4	H	801	EOT	C2-C1-C11-C12
4	H	801	EOT	N1-C1-C2-N2
4	H	801	EOT	C8-C7-N1-C1

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 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 ⓘ

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.