



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:44 AM UTC

PDB ID : 1HS6 / pdb_00001hs6
Title : STRUCTURE OF LEUKOTRIENE A4 HYDROLASE COMPLEXED WITH
BESTATIN.
Authors : Thunnissen, M.M.G.M.; Nordlund, P.N.; Haeggstrom, J.Z.
Deposited on : 2000-12-24
Resolution : 1.95 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)	:	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

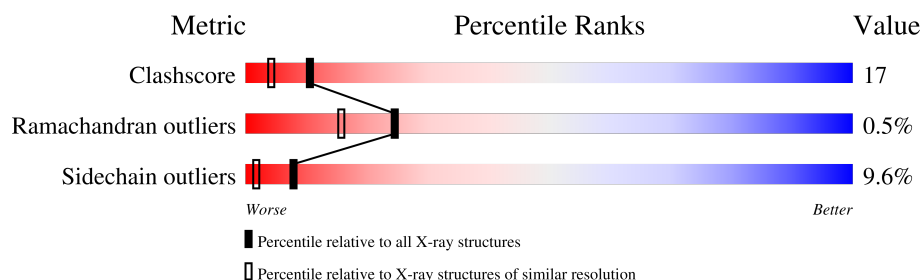
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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	A	611	 64% 28% 7%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5462 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 LEUKOTRIENE A-4 HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	610	Total	C	N	O	S	0	0	0
			4876	3130	811	914	21			

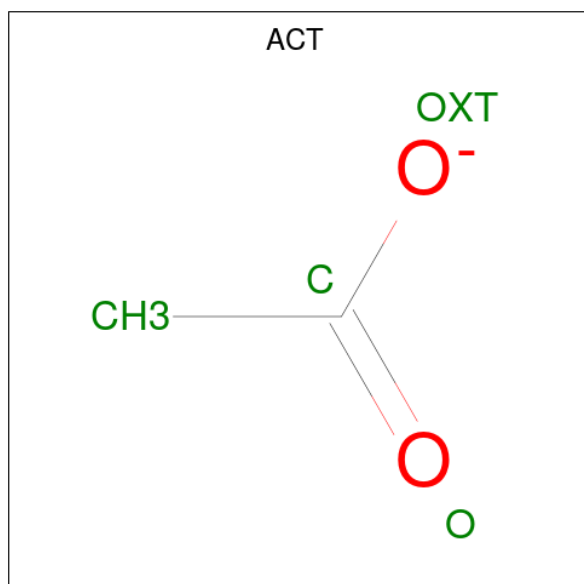
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is YTTERBIUM (III) ION (CCD ID: YB) (formula: Yb).

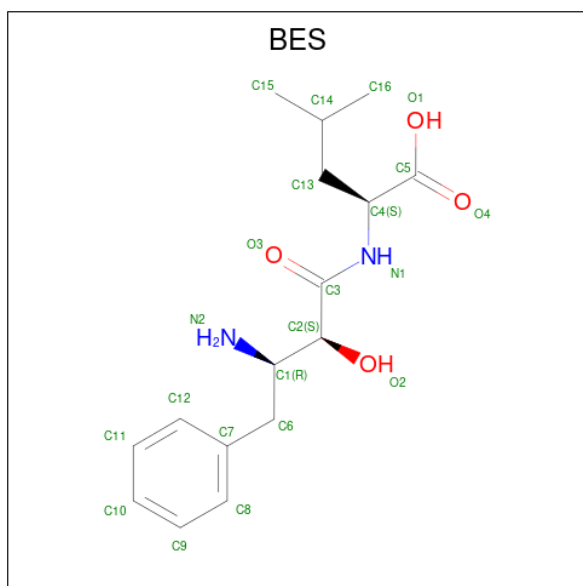
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Yb	0	0
			3	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



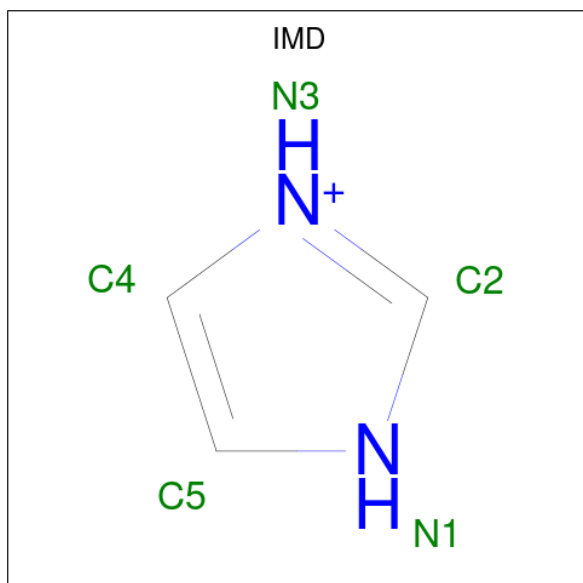
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (CCD ID: BES) (formula: $C_{16}H_{24}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			22	16	2	4		

- Molecule 6 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 7 is water.

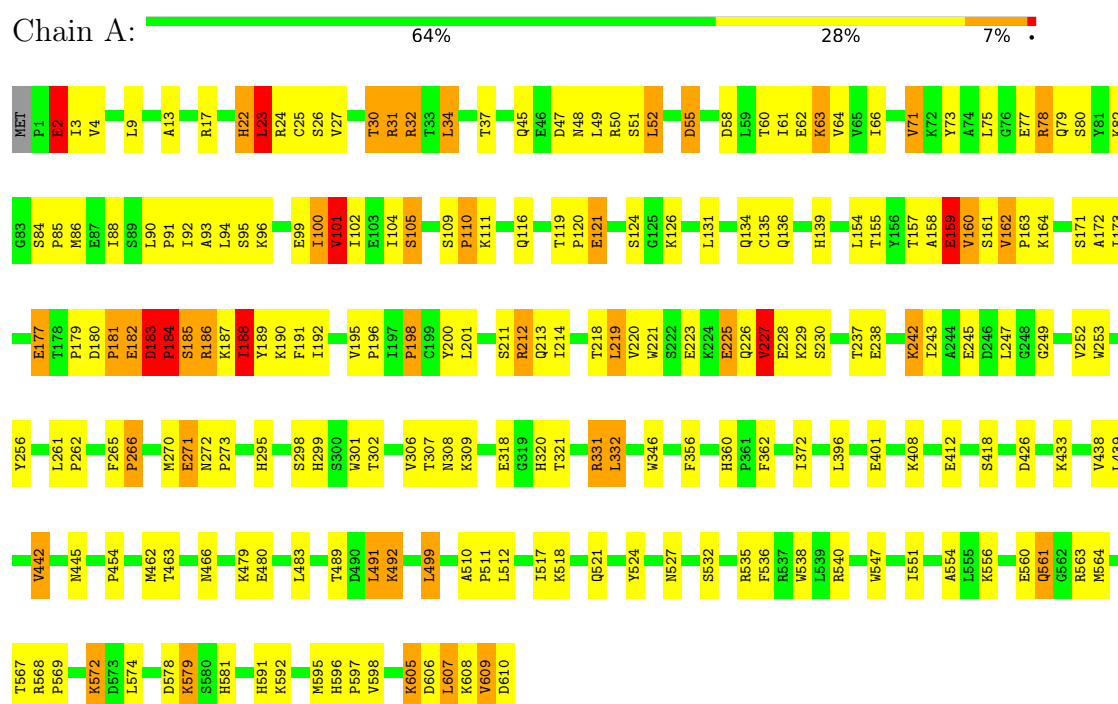
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	551	Total	O	0	0
			551	551		

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. 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: LEUKOTRIENE A-4 HYDROLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	67.60Å 133.50Å 83.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-1.95)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.188 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5462	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: ZN, IMD, BES, ACT, YB

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	0.99	0/5001	1.59	48/6798 (0.7%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ILE	CB-CA-C	10.80	125.03	110.99
1	A	180	ASP	C-N-CD	-9.62	85.55	125.00
1	A	592	LYS	N-CA-C	9.09	122.33	111.33
1	A	227	VAL	N-CA-C	8.10	118.86	110.36
1	A	2	GLU	N-CA-C	7.92	121.37	109.25
1	A	58	ASP	CA-CB-CG	-7.88	104.72	112.60
1	A	110	PRO	N-CA-CB	7.20	110.42	103.51
1	A	162	VAL	O-C-N	7.01	126.11	121.69
1	A	159	GLU	CA-C-N	-6.87	113.44	122.99
1	A	159	GLU	C-N-CA	-6.87	113.44	122.99
1	A	252	VAL	N-CA-C	6.79	119.56	112.83
1	A	4	VAL	N-CA-C	6.42	117.55	108.36
1	A	492	LYS	CA-C-N	-6.25	113.30	122.86
1	A	492	LYS	C-N-CA	-6.25	113.30	122.86
1	A	184	PRO	CB-CA-C	-6.14	101.43	111.56
1	A	101	VAL	N-CA-CB	6.07	120.39	111.52
1	A	22	HIS	N-CA-CB	5.95	119.89	110.55
1	A	237	THR	N-CA-C	5.89	118.18	111.11
1	A	223	GLU	N-CA-C	-5.80	102.84	110.43
1	A	61	ILE	CB-CA-C	-5.75	104.00	110.96
1	A	581	HIS	N-CA-C	5.68	117.95	111.02
1	A	55	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	109	SER	CA-C-N	-5.61	113.89	119.56
1	A	109	SER	C-N-CA	-5.61	113.89	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	PHE	CB-CA-C	-5.61	99.91	110.67
1	A	532	SER	N-CA-C	5.60	117.39	111.28
1	A	218	THR	N-CA-C	5.59	118.55	108.48
1	A	372	ILE	CB-CA-C	-5.57	102.32	110.62
1	A	78	ARG	CD-NE-CZ	-5.57	116.60	124.40
1	A	483	LEU	N-CA-C	5.56	118.05	111.33
1	A	183	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	567	THR	N-CA-C	5.42	116.87	111.07
1	A	196	PRO	N-CA-CB	5.40	108.11	103.36
1	A	318	GLU	N-CA-C	5.35	116.92	111.14
1	A	551	ILE	CA-C-O	5.30	122.74	118.71
1	A	134	GLN	CB-CA-C	5.27	118.78	111.51
1	A	116	GLN	N-CA-CB	5.21	118.76	110.84
1	A	273	PRO	N-CA-CB	5.19	107.94	103.27
1	A	198	PRO	N-CA-C	-5.18	103.15	111.38
1	A	85	PRO	CB-CA-C	-5.17	105.20	111.46
1	A	155	THR	N-CA-C	-5.17	102.82	110.46
1	A	266	PRO	N-CA-C	5.13	120.27	113.86
1	A	491	LEU	CA-C-N	5.12	129.33	121.19
1	A	491	LEU	C-N-CA	5.12	129.33	121.19
1	A	23	LEU	CA-C-O	5.08	125.74	120.30
1	A	426	ASP	N-CA-C	-5.07	105.75	111.28
1	A	99	GLU	N-CA-C	5.03	117.59	109.40
1	A	256	TYR	N-CA-CB	5.00	120.11	110.90

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	A	4876	0	4837	164	0
2	A	1	0	0	0	0
3	A	3	0	0	0	0
4	A	4	0	3	0	0
5	A	22	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	5	0	5	0	0
7	A	551	0	0	10	2
All	All	5462	0	4867	164	2

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 (164) 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:A:24:ARG:HG2	1:A:159:GLU:HG3	1.28	1.08
1:A:124:SER:HB3	1:A:225:GLU:HG3	1.44	0.98
1:A:360:HIS:HD2	1:A:362:PHE:H	0.94	0.93
1:A:360:HIS:CD2	1:A:362:PHE:H	1.86	0.93
1:A:184:PRO:HB2	1:A:186:ARG:HG3	1.57	0.84
1:A:62:GLU:HB3	1:A:105:SER:HB3	1.56	0.84
1:A:47:ASP:HA	1:A:95:SER:HA	1.60	0.83
1:A:295:HIS:CG	5:A:901:BES:H163	2.14	0.82
1:A:163:PRO:HD3	1:A:186:ARG:NH2	1.95	0.81
1:A:27:VAL:HG22	1:A:34:LEU:HD21	1.62	0.80
1:A:159:GLU:HB2	1:A:188:ILE:HD11	1.64	0.79
1:A:229:LYS:HG3	7:A:1501:HOH:O	1.84	0.78
1:A:17:ARG:HH11	1:A:45:GLN:HG3	1.49	0.78
1:A:32:ARG:HB2	1:A:110:PRO:HB3	1.67	0.76
1:A:572:LYS:HE2	1:A:606:ASP:CG	2.11	0.76
1:A:595:MET:HE2	7:A:1361:HOH:O	1.86	0.76
1:A:439:LEU:O	1:A:442:VAL:HG13	1.87	0.75
1:A:30:THR:HG21	1:A:31:ARG:HH21	1.51	0.74
1:A:124:SER:CB	1:A:225:GLU:HG3	2.18	0.74
1:A:182:GLU:H	1:A:184:PRO:HD3	1.54	0.73
1:A:521:GLN:HE22	1:A:527:ASN:H	1.35	0.72
1:A:163:PRO:HD3	1:A:186:ARG:CZ	2.20	0.72
1:A:30:THR:HG21	1:A:31:ARG:NH2	2.05	0.71
1:A:13:ALA:O	1:A:17:ARG:NH1	2.24	0.70
1:A:24:ARG:HG2	1:A:159:GLU:CG	2.14	0.70
1:A:164:LYS:HG3	1:A:185:SER:O	1.92	0.70
1:A:48:ASN:N	1:A:94:LEU:O	2.25	0.69
1:A:183:ASP:N	1:A:184:PRO:HD3	2.07	0.68
1:A:100:ILE:CD1	1:A:102:ILE:HD11	2.23	0.68
1:A:605:LYS:HE3	7:A:1239:HOH:O	1.93	0.68
1:A:17:ARG:NH1	1:A:45:GLN:HG3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:THR:OG1	1:A:121:GLU:HG2	1.95	0.66
1:A:22:HIS:CE1	1:A:24:ARG:HG3	2.31	0.65
1:A:466:ASN:ND2	7:A:1481:HOH:O	2.27	0.65
1:A:331:ARG:HG2	1:A:331:ARG:HH11	1.60	0.65
1:A:17:ARG:HH11	1:A:45:GLN:CG	2.11	0.64
1:A:445:ASN:HB2	7:A:1378:HOH:O	1.98	0.63
1:A:225:GLU:H	1:A:225:GLU:CD	2.05	0.63
1:A:162:VAL:HA	1:A:186:ARG:NH2	2.13	0.63
1:A:568:ARG:HB2	1:A:569:PRO:HD3	1.81	0.63
1:A:238:GLU:OE2	1:A:242:LYS:HD2	2.00	0.61
1:A:49:LEU:HB3	1:A:94:LEU:HB2	1.82	0.61
1:A:182:GLU:C	1:A:184:PRO:HD3	2.25	0.61
1:A:596:HIS:CD2	1:A:598:VAL:H	2.19	0.61
1:A:227:VAL:HG12	1:A:228:GLU:N	2.15	0.61
1:A:100:ILE:HD13	1:A:102:ILE:HD11	1.82	0.61
1:A:360:HIS:HD2	1:A:362:PHE:N	1.80	0.61
1:A:23:LEU:O	1:A:158:ALA:HA	2.02	0.60
1:A:261:LEU:HB3	1:A:262:PRO:HD2	1.82	0.60
1:A:198:PRO:HD2	1:A:201:LEU:HD12	1.85	0.59
1:A:214:ILE:HD13	1:A:220:VAL:HG22	1.85	0.58
1:A:27:VAL:O	1:A:186:ARG:NH2	2.35	0.58
1:A:94:LEU:HD11	1:A:100:ILE:HG13	1.85	0.58
1:A:37:THR:HA	1:A:104:ILE:O	2.03	0.58
1:A:211:SER:HA	1:A:220:VAL:O	2.04	0.58
1:A:211:SER:HB3	1:A:221:TRP:CE3	2.39	0.57
1:A:214:ILE:HD13	1:A:220:VAL:CG2	2.35	0.56
1:A:572:LYS:HE2	1:A:606:ASP:OD2	2.05	0.56
1:A:30:THR:CG2	1:A:31:ARG:HH21	2.17	0.56
1:A:261:LEU:HB3	1:A:262:PRO:CD	2.36	0.56
1:A:47:ASP:OD1	1:A:96:LYS:HG3	2.07	0.55
1:A:17:ARG:HH11	1:A:45:GLN:CD	2.14	0.55
1:A:396:LEU:HG	1:A:438:VAL:CG1	2.36	0.55
1:A:331:ARG:HH11	1:A:331:ARG:CG	2.19	0.54
1:A:100:ILE:HD13	1:A:102:ILE:CG1	2.38	0.53
1:A:243:ILE:HD11	1:A:332:LEU:HD13	1.91	0.53
1:A:596:HIS:HD2	1:A:598:VAL:H	1.55	0.52
1:A:95:SER:O	1:A:96:LYS:C	2.49	0.52
1:A:521:GLN:NE2	1:A:527:ASN:H	2.06	0.51
1:A:527:ASN:ND2	1:A:538:TRP:HE1	2.08	0.51
1:A:161:SER:OG	1:A:186:ARG:HB2	2.10	0.51
1:A:298:SER:HB2	1:A:321:THR:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:NH1	1:A:45:GLN:NE2	2.59	0.50
1:A:177:GLU:HG3	1:A:177:GLU:O	2.11	0.50
1:A:86:MET:HE2	1:A:88:ILE:HD11	1.93	0.50
1:A:607:LEU:O	1:A:608:LYS:HB2	2.12	0.50
1:A:51:SER:HA	1:A:90:LEU:HG	1.93	0.50
1:A:64:VAL:HG12	1:A:71:VAL:HG22	1.93	0.50
1:A:561:GLN:NE2	1:A:563:ARG:H	2.10	0.50
1:A:331:ARG:CG	1:A:331:ARG:NH1	2.74	0.49
1:A:183:ASP:N	1:A:184:PRO:CD	2.74	0.49
1:A:212:ARG:CZ	1:A:227:VAL:HG11	2.42	0.49
1:A:192:ILE:HD12	1:A:192:ILE:O	2.12	0.49
1:A:302:THR:HG21	1:A:320:HIS:HB3	1.95	0.49
1:A:607:LEU:HB3	1:A:609:VAL:CG1	2.43	0.49
1:A:518:LYS:HE2	1:A:547:TRP:NE1	2.28	0.49
1:A:243:ILE:CD1	1:A:332:LEU:HD13	2.43	0.49
1:A:489:THR:O	1:A:492:LYS:HB2	2.13	0.49
1:A:527:ASN:HD22	1:A:538:TRP:HE1	1.59	0.48
1:A:24:ARG:HD2	7:A:1619:HOH:O	2.13	0.48
1:A:100:ILE:HD11	1:A:102:ILE:HD11	1.96	0.48
1:A:578:ASP:OD1	1:A:579:LYS:HG2	2.14	0.48
1:A:120:PRO:O	1:A:126:LYS:HA	2.14	0.48
1:A:265:PHE:CD1	1:A:266:PRO:HD2	2.49	0.48
1:A:100:ILE:HD13	1:A:102:ILE:CD1	2.44	0.47
1:A:554:ALA:HB3	1:A:574:LEU:HD21	1.96	0.47
1:A:401:GLU:HB2	7:A:1650:HOH:O	2.13	0.47
1:A:214:ILE:CD1	1:A:220:VAL:HG22	2.43	0.47
1:A:82:LYS:HE3	7:A:1119:HOH:O	2.15	0.47
1:A:163:PRO:HD3	1:A:186:ARG:HH22	1.76	0.47
1:A:182:GLU:N	1:A:184:PRO:HD3	2.25	0.47
1:A:2:GLU:OE1	1:A:2:GLU:HA	2.13	0.47
1:A:220:VAL:HG11	1:A:230:SER:HB3	1.97	0.47
1:A:510:ALA:HB1	1:A:511:PRO:HA	1.96	0.47
1:A:295:HIS:CB	5:A:901:BES:H163	2.44	0.46
1:A:92:ILE:HG22	1:A:93:ALA:O	2.15	0.46
1:A:52:LEU:CD1	1:A:90:LEU:HD21	2.46	0.46
1:A:213:GLN:HA	1:A:219:LEU:HA	1.98	0.46
1:A:591:HIS:CB	1:A:595:MET:HE3	2.45	0.46
1:A:9:LEU:N	1:A:55:ASP:OD1	2.34	0.46
1:A:226:GLN:HG2	7:A:1461:HOH:O	2.16	0.45
1:A:52:LEU:HD13	1:A:90:LEU:HD21	1.97	0.45
1:A:172:ALA:HB3	1:A:191:PHE:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HA	1:A:75:LEU:HD23	1.83	0.45
1:A:136:GLN:OE1	1:A:270:MET:HE1	2.16	0.45
1:A:491:LEU:HD11	1:A:524:TYR:HB3	1.98	0.45
1:A:159:GLU:HA	1:A:189:TYR:O	2.17	0.45
1:A:171:SER:HB3	1:A:272:ASN:HB3	1.99	0.45
1:A:213:GLN:HB2	1:A:219:LEU:CD1	2.47	0.44
1:A:26:SER:OG	1:A:161:SER:HB3	2.18	0.44
1:A:161:SER:HA	1:A:187:LYS:O	2.18	0.44
1:A:163:PRO:HD3	1:A:186:ARG:NH1	2.32	0.44
1:A:50:ARG:HE	1:A:93:ALA:HB2	1.82	0.44
1:A:499:LEU:HD12	1:A:499:LEU:HA	1.69	0.44
1:A:596:HIS:CG	1:A:597:PRO:HD2	2.53	0.44
1:A:78:ARG:HH11	1:A:78:ARG:HD2	1.50	0.43
1:A:396:LEU:HG	1:A:438:VAL:HG12	2.00	0.43
1:A:479:LYS:O	1:A:480:GLU:C	2.58	0.43
1:A:536:PHE:CZ	1:A:540:ARG:HD2	2.53	0.43
1:A:535:ARG:O	1:A:536:PHE:C	2.59	0.43
1:A:34:LEU:HA	1:A:34:LEU:HD23	1.56	0.43
1:A:26:SER:OG	1:A:186:ARG:NE	2.52	0.43
1:A:27:VAL:HG22	1:A:34:LEU:CD2	2.41	0.43
1:A:346:TRP:CZ3	1:A:454:PRO:HG2	2.54	0.43
1:A:48:ASN:HA	1:A:93:ALA:HB1	2.01	0.42
1:A:63:LYS:HG2	1:A:105:SER:HB2	2.01	0.42
1:A:609:VAL:O	1:A:610:ASP:HB2	2.20	0.42
1:A:195:VAL:HB	1:A:253:TRP:CZ3	2.53	0.42
1:A:245:GLU:HA	1:A:249:GLY:O	2.19	0.42
1:A:135:CYS:HA	1:A:139:HIS:HB2	2.00	0.42
1:A:163:PRO:CD	1:A:186:ARG:NH2	2.76	0.42
1:A:173:ILE:O	1:A:191:PHE:HA	2.20	0.42
1:A:164:LYS:HA	1:A:187:LYS:HG3	2.02	0.42
1:A:307:THR:O	1:A:418:SER:HA	2.20	0.42
1:A:30:THR:CG2	1:A:31:ARG:NH2	2.78	0.42
1:A:266:PRO:HB2	1:A:564:MET:HE2	2.01	0.42
1:A:25:CYS:O	1:A:160:VAL:HA	2.20	0.41
1:A:90:LEU:HA	1:A:91:PRO:HD3	1.94	0.41
1:A:212:ARG:NE	1:A:227:VAL:HG11	2.35	0.41
1:A:556:LYS:HE3	1:A:560:GLU:OE1	2.20	0.41
1:A:179:PRO:O	1:A:181:PRO:HD3	2.19	0.41
1:A:198:PRO:HB2	1:A:200:TYR:CD2	2.55	0.41
1:A:579:LYS:HG3	7:A:1523:HOH:O	2.19	0.41
1:A:591:HIS:CB	1:A:595:MET:CE	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:HG22	1:A:192:ILE:HG22	2.03	0.41
1:A:66:ILE:HG23	1:A:101:VAL:O	2.21	0.41
1:A:162:VAL:HA	1:A:186:ARG:HH21	1.82	0.41
1:A:164:LYS:HD2	1:A:185:SER:OG	2.21	0.41
1:A:512:LEU:HB2	1:A:517:ILE:HD11	2.02	0.41
1:A:73:TYR:CD1	1:A:73:TYR:C	2.99	0.41
1:A:79:GLN:O	1:A:80:SER:C	2.64	0.41
1:A:271:GLU:OE1	5:A:901:BES:N2	2.54	0.40
1:A:299:HIS:C	1:A:301:TRP:N	2.79	0.40
1:A:462:MET:O	1:A:463:THR:C	2.63	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1493:HOH:O	7:A:1493:HOH:O[2_665]	0.57	1.63
7:A:1652:HOH:O	7:A:1652:HOH:O[2_665]	1.46	0.74

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	A	608/611 (100%)	580 (95%)	25 (4%)	3 (0%)	24 16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	PRO
1	A	184	PRO
1	A	271	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	542/543 (100%)	490 (90%)	52 (10%)	8 2

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	ILE
1	A	23	LEU
1	A	30	THR
1	A	31	ARG
1	A	32	ARG
1	A	34	LEU
1	A	52	LEU
1	A	60	THR
1	A	63	LYS
1	A	71	VAL
1	A	77	GLU
1	A	84	SER
1	A	100	ILE
1	A	101	VAL
1	A	105	SER
1	A	111	LYS
1	A	121	GLU
1	A	131	LEU
1	A	154	LEU
1	A	159	GLU
1	A	160	VAL
1	A	177	GLU
1	A	182	GLU
1	A	183	ASP
1	A	184	PRO
1	A	185	SER
1	A	186	ARG
1	A	188	ILE
1	A	190	LYS

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Mol	Chain	Res	Type
1	A	212	ARG
1	A	219	LEU
1	A	225	GLU
1	A	227	VAL
1	A	242	LYS
1	A	247	LEU
1	A	306	VAL
1	A	308	ASN
1	A	309	LYS
1	A	331	ARG
1	A	332	LEU
1	A	408	LYS
1	A	412	GLU
1	A	433	LYS
1	A	442	VAL
1	A	499	LEU
1	A	561	GLN
1	A	572	LYS
1	A	579	LYS
1	A	605	LYS
1	A	607	LEU
1	A	609	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	43	GLN
1	A	45	GLN
1	A	69	GLN
1	A	116	GLN
1	A	213	GLN
1	A	226	GLN
1	A	291	ASN
1	A	341	ASN
1	A	350	GLN
1	A	360	HIS
1	A	440	ASN
1	A	459	ASN
1	A	466	ASN
1	A	521	GLN
1	A	525	ASN

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Mol	Chain	Res	Type
1	A	527	ASN
1	A	561	GLN
1	A	596	HIS

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	ACT	A	1101	-	3,3,3	0.58	0	3,3,3	1.60	1 (33%)
5	BES	A	901	2	22,22,22	0.58	0	26,29,29	0.96	1 (3%)
6	IMD	A	1001	-	5,5,5	0.38	0	5,5,5	0.71	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
5	BES	A	901	2	-	6/24/24/24	0/1/1/1
6	IMD	A	1001	-	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	BES	C2-C3-N1	-2.29	113.12	116.22
4	A	1101	ACT	OXT-C-CH3	-2.16	106.00	115.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

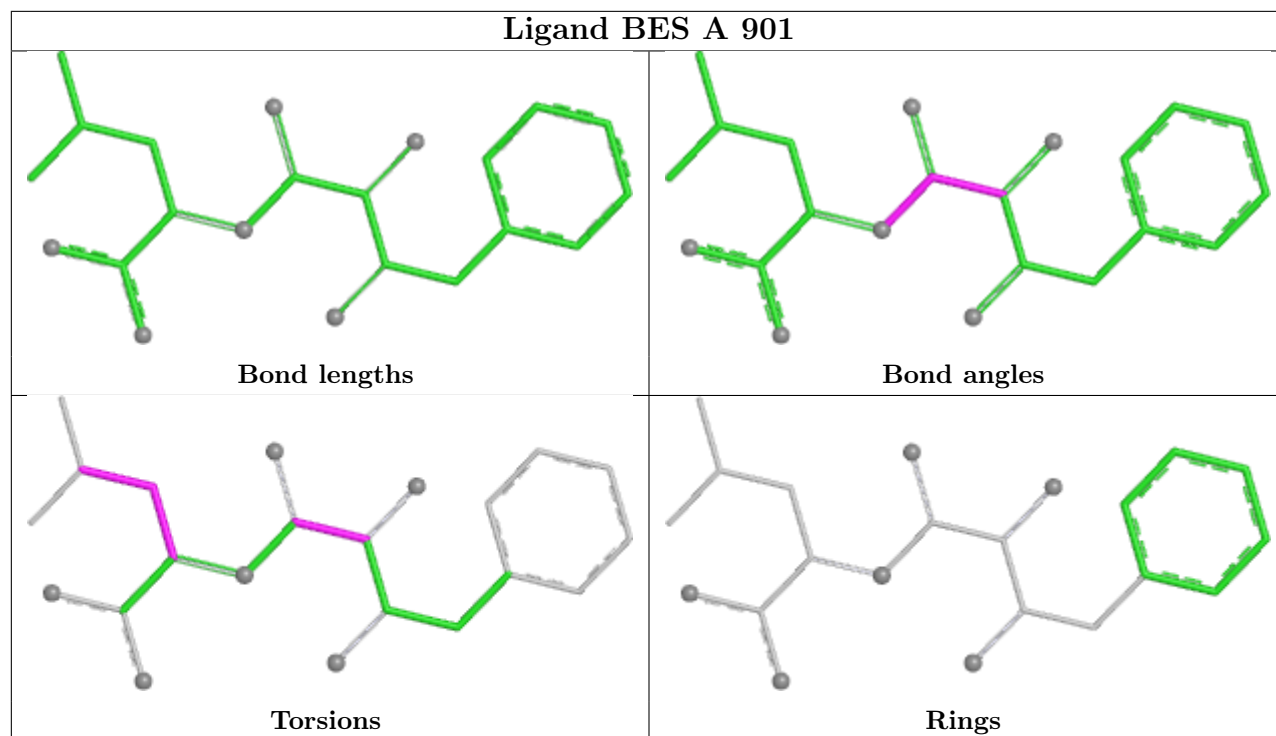
Mol	Chain	Res	Type	Atoms
5	A	901	BES	O2-C2-C3-N1
5	A	901	BES	C14-C13-C4-C5
5	A	901	BES	C14-C13-C4-N1
5	A	901	BES	C4-C13-C14-C15
5	A	901	BES	O2-C2-C3-O3
5	A	901	BES	C4-C13-C14-C16

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	BES	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.