



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:48 PM GMT

PDB ID : 1HS6
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

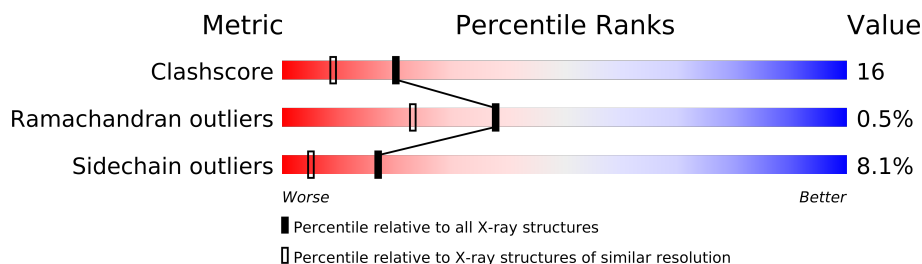
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	611	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5462 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

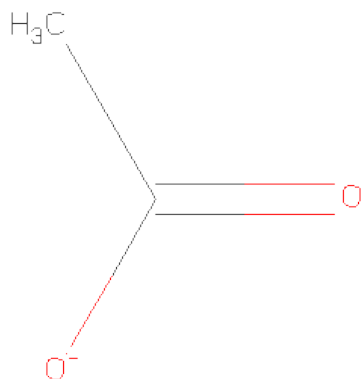
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

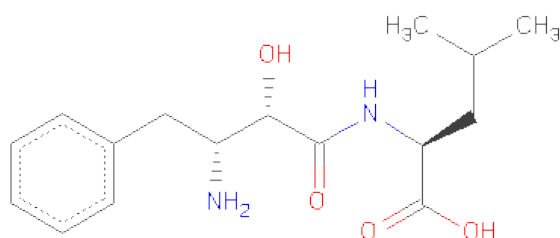
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Yb	0	0
			3	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



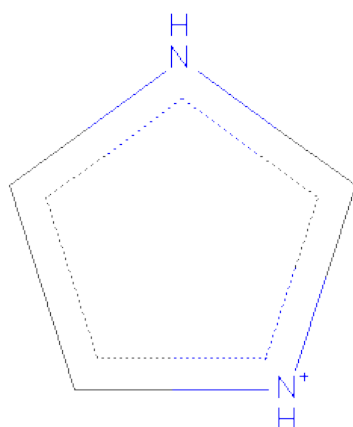
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOICACID (three-letter code: BES) (formula: C₁₆H₂₄N₂O₄).



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

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



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

- Molecule 7 is water.

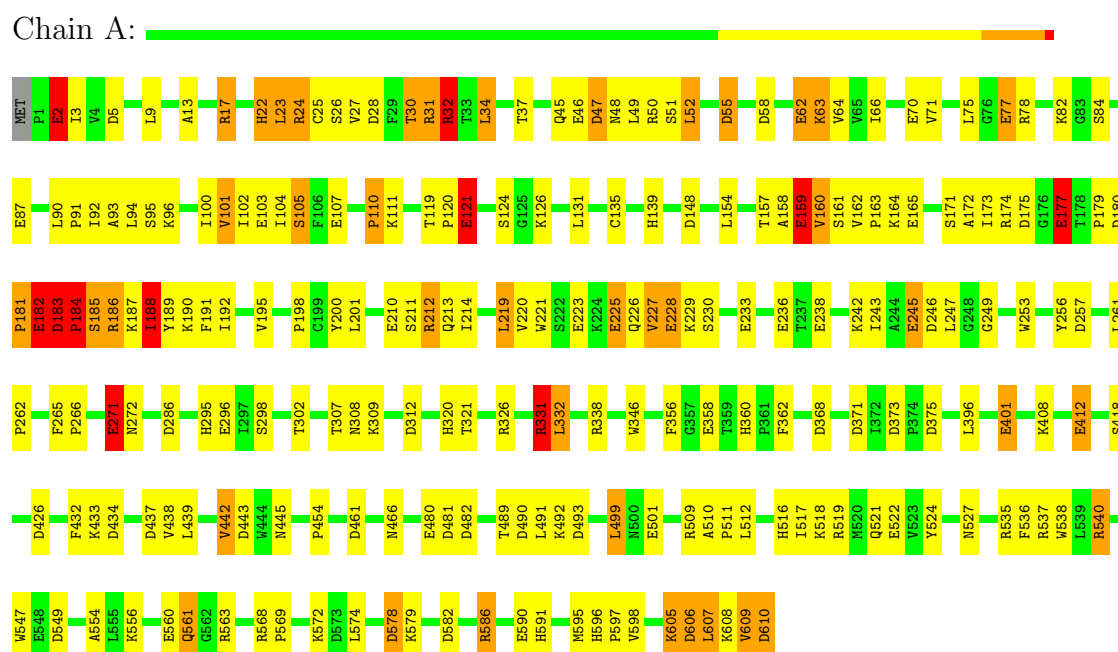
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	551	Total	O	0	0
			551	551		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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 will therefore be 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: BES, ZN, YB, IMD, ACT

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	0.89	29/5001 (0.6%)	1.40	75/6798 (1.1%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	GLU	CD-OE2	6.43	1.32	1.25
1	A	62	GLU	CD-OE2	6.39	1.32	1.25
1	A	233	GLU	CD-OE2	6.34	1.32	1.25
1	A	77	GLU	CD-OE2	6.32	1.32	1.25
1	A	2	GLU	CD-OE2	6.16	1.32	1.25
1	A	296	GLU	CD-OE2	6.16	1.32	1.25
1	A	590	GLU	CD-OE2	6.15	1.32	1.25
1	A	245	GLU	CD-OE2	5.96	1.32	1.25
1	A	103	GLU	CD-OE2	5.91	1.32	1.25
1	A	177	GLU	CD-OE2	5.90	1.32	1.25
1	A	46	GLU	CD-OE2	5.88	1.32	1.25
1	A	412	GLU	CD-OE2	5.86	1.32	1.25
1	A	223	GLU	CD-OE2	5.86	1.32	1.25
1	A	358	GLU	CD-OE2	5.85	1.32	1.25
1	A	501	GLU	CD-OE2	5.82	1.32	1.25
1	A	165	GLU	CD-OE2	5.80	1.32	1.25
1	A	182	GLU	CD-OE2	5.73	1.31	1.25
1	A	121	GLU	CD-OE2	5.64	1.31	1.25
1	A	228	GLU	CD-OE2	5.61	1.31	1.25
1	A	70	GLU	CD-OE2	5.51	1.31	1.25
1	A	225	GLU	CD-OE2	5.45	1.31	1.25
1	A	480	GLU	CD-OE2	5.43	1.31	1.25
1	A	87	GLU	CD-OE2	5.39	1.31	1.25
1	A	159	GLU	CD-OE2	5.38	1.31	1.25
1	A	210	GLU	CD-OE2	5.31	1.31	1.25
1	A	522	GLU	CD-OE2	5.26	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLU	CD-OE2	5.22	1.31	1.25
1	A	271	GLU	CD-OE2	5.16	1.31	1.25
1	A	107	GLU	CD-OE2	5.08	1.31	1.25

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASP	C-N-CD	-15.93	85.55	120.60
1	A	509	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	A	481	ASP	CB-CG-OD1	10.15	127.44	118.30
1	A	371	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	A	578	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	A	338	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	175	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	A	481	ASP	CB-CG-OD2	-8.43	110.71	118.30
1	A	55	ASP	CB-CG-OD2	-8.14	110.98	118.30
1	A	434	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	331	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	A	55	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	437	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	A	509	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	368	ASP	CB-CG-OD1	7.36	124.93	118.30
1	A	443	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	A	578	ASP	CB-CG-OD1	7.26	124.83	118.30
1	A	47	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	A	28	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	432	PHE	CB-CG-CD2	6.96	125.67	120.80
1	A	373	ASP	CB-CG-OD1	6.95	124.56	118.30
1	A	434	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	A	24	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	549	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	493	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	490	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	246	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	A	246	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	188	ILE	CB-CA-C	6.71	125.03	111.60
1	A	28	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	148	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	312	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	257	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	175	ASP	CB-CG-OD1	6.47	124.13	118.30
1	A	535	ARG	NE-CZ-NH1	6.44	123.52	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	ASP	CB-CG-OD1	6.42	124.07	118.30
1	A	174	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	432	PHE	CB-CG-CD1	-6.41	116.32	120.80
1	A	257	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	148	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	373	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	606	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	482	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	58	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	586	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	5	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	110	PRO	N-CA-CB	5.93	110.42	103.30
1	A	461	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	32	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	606	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	312	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	490	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	183	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	375	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	326	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	442	VAL	CG1-CB-CG2	5.64	119.92	110.90
1	A	286	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	437	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	540	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	519	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	286	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	A	368	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	582	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	183	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	537	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	17	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	482	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	535	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	256	TYR	N-CA-CB	5.28	120.11	110.60
1	A	219	LEU	CB-CA-C	-5.27	100.18	110.20
1	A	356	PHE	CB-CA-C	-5.25	99.91	110.40
1	A	461	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	610	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	22	HIS	N-CA-CB	5.16	119.89	110.60
1	A	426	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4876	0	4837	155	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
6	A	5	0	5	0	0
7	A	551	0	0	9	2
All	All	5462	0	4867	155	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (155) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:591:HIS:HB3	1:A:595:MET:HE2	1.69	0.72
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:572:LYS:HE2	1:A:606:ASP:CG	2.11	0.71
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
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:HH11	1:A:331:ARG:HG2	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:162:VAL:HA	1:A:186:ARG:NH2	2.13	0.63
1:A:591:HIS:CB	1:A:595:MET:HE2	2.28	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: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:360:HIS:HD2	1:A:362:PHE:N	1.80	0.61
1:A:100:ILE:HD13	1:A:102:ILE:HD11	1.82	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:225:GLU:CD	1:A:225:GLU:H	2.05	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:211:SER:HA	1:A:220:VAL:O	2.04	0.58
1:A:37:THR:HA	1:A:104:ILE:O	2.03	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:182:GLU:C	1:A:184:PRO:HD3	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:396:LEU:HG	1:A:438:VAL:CG1	2.36	0.55
1:A:331:ARG:CG	1:A:331:ARG:HH11	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: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
1:A:17:ARG:HH11	1:A:45:GLN:CD	2.14	0.50
1:A:17:ARG:NH1	1:A:45:GLN:NE2	2.59	0.50
1:A:177:GLU:O	1:A:177:GLU:HG3	2.11	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:561:GLN:NE2	1:A:563:ARG:H	2.10	0.50
1:A:64:VAL:HG12	1:A:71:VAL:HG22	1.93	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:607:LEU:HB3	1:A:609:VAL:CG1	2.43	0.49
1:A:302:THR:HG21	1:A:320:HIS:HB3	1.95	0.49
1:A:192:ILE:O	1:A:192:ILE:HD12	2.12	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:95:SER:O	1:A:96:LYS:C	2.49	0.47
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:220:VAL:HG11	1:A:230:SER:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:510:ALA:HB1	1:A:511:PRO:HA	1.96	0.47
1:A:2:GLU:OE1	1:A:2:GLU:HA	2.13	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: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
1:A:491:LEU:HD11	1:A:524:TYR:HB3	1.98	0.45
1:A:75:LEU:HA	1:A:75:LEU:HD23	1.83	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:163:PRO:HD3	1:A:186:ARG:NH1	2.32	0.44
1:A:161:SER:HA	1:A:187:LYS:O	2.18	0.44
1:A:26:SER:OG	1:A:161:SER:HB3	2.18	0.44
1:A:50:ARG:HE	1:A:93:ALA:HB2	1.82	0.44
1:A:499:LEU:HA	1:A:499:LEU:HD12	1.69	0.44
1:A:596:HIS:CG	1:A:597:PRO:HD2	2.53	0.44
1:A:396:LEU:HG	1:A:438:VAL:HG12	2.00	0.43
1:A:78:ARG:HD2	1:A:78:ARG:HH11	1.50	0.43
1:A:536:PHE:CZ	1:A:540:ARG:HD2	2.53	0.43
1:A:34:LEU:HD23	1:A:34:LEU:HA	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:245:GLU:HA	1:A:249:GLY:O	2.19	0.42
1:A:195:VAL:HB	1:A:253:TRP:CZ3	2.53	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:135:CYS:HA	1:A:139:HIS:HB2	2.00	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:212:ARG:NE	1:A:227:VAL:HG11	2.35	0.41
1:A:90:LEU:HA	1:A:91:PRO:HD3	1.94	0.41
1:A:25:CYS:O	1:A:160:VAL:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:556:LYS:HE3	1:A:560:GLU:OE1	2.20	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:179:PRO:O	1:A:181:PRO:HD3	2.19	0.41
1:A:591:HIS:CB	1:A:595:MET:CE	2.98	0.41
1:A:157:THR:HG22	1:A:192:ILE:HG22	2.03	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:66:ILE:HG23	1:A:101:VAL:O	2.21	0.41
1:A:512:LEU:HB2	1:A:517:ILE:HD11	2.02	0.41
1:A:271:GLU:OE1	5:A:901:BES:N2	2.54	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	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	608/611 (100%)	580 (95%)	25 (4%)	3 (0%)	38 23

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%)	498 (92%)	44 (8%)	17 5

All (44) 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	63	LYS
1	A	77	GLU
1	A	84	SER
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
1	A	212	ARG
1	A	227	VAL
1	A	247	LEU
1	A	308	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	499	LEU
1	A	516	HIS
1	A	561	GLN
1	A	586	ARG
1	A	605	LYS
1	A	607	LEU
1	A	609	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	43	GLN
1	A	45	GLN
1	A	213	GLN
1	A	226	GLN
1	A	341	ASN
1	A	350	GLN
1	A	360	HIS
1	A	440	ASN
1	A	441	GLN
1	A	445	ASN
1	A	466	ASN
1	A	521	GLN
1	A	525	ASN
1	A	527	ASN
1	A	544	GLN
1	A	561	GLN
1	A	596	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	$\# Z > 2$
6	IMD	A	1001	-	5,5,5	0.81	0	5,5,5	0.51	0
4	ACT	A	1101	-	1,3,3	1.01	0	0,3,3	0.00	-
5	BES	A	901	2	22,22,22	0.57	0	29,29,29	0.91	1 (3%)

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
6	IMD	A	1001	-	-	0/0/0/0	0/1/1/1
4	ACT	A	1101	-	-	0/0/0/0	0/0/0/0
5	BES	A	901	2	-	0/24/24/24	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	BES	C2-C3-N1	-2.26	113.12	116.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.