



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1W50 / pdb_00001w50
Title : Apo Structure of BACE (Beta Secretase)
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Deposited on : 2004-08-04
Resolution : 1.75 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

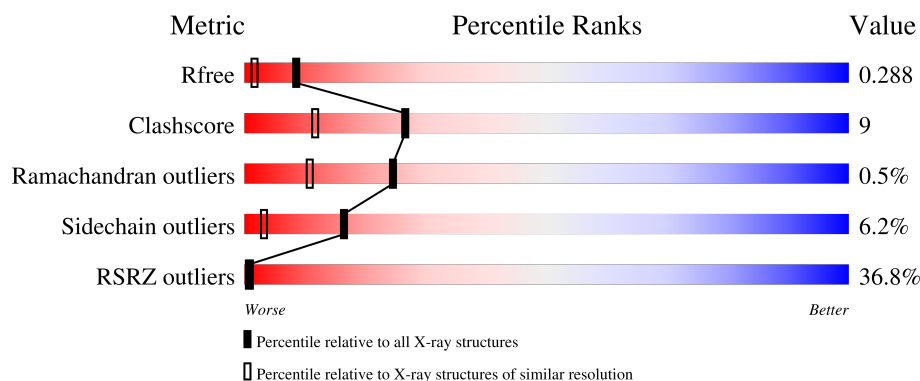
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	411	34% 77% 13% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3249 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 BETA-SECRETASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	26	0	1
			2966	1898	494	560	14			

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	I	0	0
			4	4		

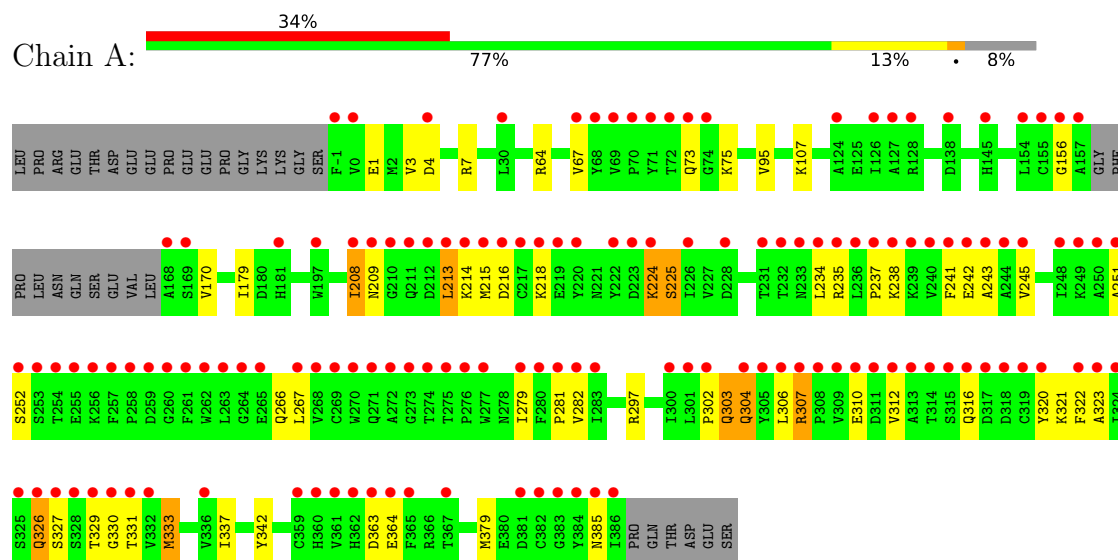
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	279	Total	O	0	0
			279	279		

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 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.

• Molecule 1: BETA-SECRETASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	103.24Å 103.24Å 169.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.52 – 1.75 39.52 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.1 (39.52-1.75) 95.1 (39.52-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.1.29	Depositor
R, R_{free}	0.244 , 0.283 0.248 , 0.288	Depositor DCC
R_{free} test set	2624 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3249	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.94	6/3041 (0.2%)	0.97	4/4134 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ARG	CD-NE	16.55	1.69	1.46
1	A	7	ARG	CD-NE	-12.25	1.29	1.46
1	A	1	GLU	CB-CG	-11.28	1.18	1.52
1	A	333	MET	SD-CE	-8.48	1.58	1.79
1	A	379	MET	SD-CE	-7.31	1.61	1.79
1	A	385	ASN	C-N	-6.88	1.23	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	CD-NE-CZ	-10.00	110.40	124.40
1	A	7	ARG	CD-NE-CZ	8.39	136.14	124.40
1	A	7	ARG	CG-CD-NE	7.32	128.10	112.00
1	A	385	ASN	O-C-N	-5.20	114.69	123.00

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	A	2966	0	2878	52	0
2	A	4	0	0	2	0
3	A	279	0	0	27	0
All	All	3249	0	2878	54	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 9.

All (54) 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:A:1505:IOD:I	3:A:2088:HOH:O	2.35	1.13
1:A:304:GLN:HE21	1:A:304:GLN:N	1.53	1.06
2:A:1503:IOD:I	3:A:2122:HOH:O	2.51	0.99
1:A:237:PRO:HA	3:A:2253:HOH:O	1.69	0.90
1:A:251:ALA:HB3	3:A:2214:HOH:O	1.74	0.88
1:A:281:PRO:C	3:A:2226:HOH:O	2.18	0.86
1:A:330:GLY:O	3:A:2254:HOH:O	1.95	0.84
1:A:303:GLN:C	1:A:304:GLN:HE21	1.94	0.74
1:A:281:PRO:HD3	3:A:2219:HOH:O	1.87	0.73
1:A:242:GLU:HG2	3:A:2251:HOH:O	1.89	0.72
1:A:252:SER:HB3	3:A:2219:HOH:O	1.90	0.69
1:A:215:MET:CE	1:A:243:ALA:HB3	2.26	0.65
1:A:73:GLN:O	1:A:107:LYS:HD2	1.97	0.65
1:A:326:GLN:NE2	3:A:2251:HOH:O	2.31	0.63
1:A:282:VAL:N	3:A:2226:HOH:O	2.29	0.62
1:A:330:GLY:N	3:A:2198:HOH:O	2.32	0.61
1:A:235:ARG:HB3	1:A:327:SER:OG	2.00	0.60
1:A:224:LYS:NZ	3:A:2200:HOH:O	2.33	0.60
1:A:224:LYS:NZ	1:A:329:THR:O	2.29	0.59
1:A:333:MET:HE2	1:A:337:ILE:HG21	1.85	0.59
1:A:279:ILE:HG23	3:A:2218:HOH:O	2.06	0.56
1:A:208:ILE:HD12	1:A:213:LEU:HD11	1.88	0.55
1:A:225:SER:HB2	3:A:2201:HOH:O	2.06	0.55
1:A:215:MET:HE2	1:A:243:ALA:HB3	1.87	0.55
1:A:156:GLY:HA2	1:A:170:VAL:HG12	1.88	0.54
1:A:235:ARG:HB3	1:A:327:SER:HG	1.72	0.54
1:A:303:GLN:C	1:A:304:GLN:NE2	2.63	0.54
1:A:215:MET:HE1	1:A:243:ALA:HB3	1.91	0.53
1:A:215:MET:O	1:A:216:ASP:C	2.51	0.53
1:A:307:ARG:HD3	1:A:323:ALA:HB2	1.94	0.50
1:A:225:SER:OG	1:A:331:THR:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:HE2	1:A:243:ALA:CB	2.41	0.50
1:A:304:GLN:HE21	1:A:304:GLN:CA	2.21	0.49
1:A:329:THR:C	3:A:2198:HOH:O	2.56	0.48
1:A:252:SER:N	3:A:2219:HOH:O	2.46	0.48
1:A:333:MET:CE	1:A:337:ILE:HG21	2.43	0.48
1:A:302:PRO:O	1:A:306:LEU:HB2	2.14	0.48
1:A:156:GLY:HA2	1:A:170:VAL:CB	2.44	0.47
1:A:3:VAL:O	1:A:4:ASP:CG	2.59	0.45
1:A:156:GLY:HA2	1:A:170:VAL:CG1	2.46	0.45
1:A:224:LYS:O	1:A:331:THR:N	2.44	0.45
1:A:321:LYS:C	3:A:2248:HOH:O	2.59	0.45
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.82	0.44
1:A:156:GLY:HA2	1:A:170:VAL:HB	1.99	0.44
1:A:241:PHE:CZ	1:A:245:VAL:HG21	2.53	0.43
1:A:364:GLU:HB3	3:A:2262:HOH:O	2.17	0.43
1:A:303:GLN:OE1	3:A:2240:HOH:O	2.21	0.42
1:A:107:LYS:HA	3:A:2125:HOH:O	2.19	0.42
1:A:320:TYR:HB3	3:A:2248:HOH:O	2.19	0.41
1:A:235:ARG:C	3:A:2254:HOH:O	2.63	0.41
1:A:322:PHE:HA	3:A:2249:HOH:O	2.20	0.41
1:A:327:SER:C	3:A:2253:HOH:O	2.65	0.40
1:A:225:SER:N	3:A:2201:HOH:O	2.53	0.40
1:A:297:ARG:HG3	3:A:2237:HOH:O	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	A	374/411 (91%)	355 (95%)	17 (4%)	2 (0%)	24 11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	GLU
1	A	363	ASP

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	321/352 (91%)	301 (94%)	20 (6%)	16 3

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	75	LYS
1	A	95	VAL
1	A	208	ILE
1	A	209	ASN
1	A	213	LEU
1	A	214	LYS
1	A	218	LYS
1	A	224	LYS
1	A	225	SER
1	A	234	LEU
1	A	238	LYS
1	A	266	GLN
1	A	267	LEU
1	A	303	GLN
1	A	304	GLN
1	A	307	ARG
1	A	312	VAL
1	A	316	GLN
1	A	326	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	211	GLN
1	A	278	ASN
1	A	304	GLN
1	A	326	GLN
1	A	360	HIS
1	A	385	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	378/411 (91%)	1.85	139 (36%) ⓘ ⓘ	15, 30, 64, 94	11 (2%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	ILE	8.9
1	A	312	VAL	7.7
1	A	277	TRP	7.4
1	A	319	CYS	7.3
1	A	257	PHE	7.1
1	A	365	PHE	7.0
1	A	313	ALA	6.7
1	A	245	VAL	6.6
1	A	270	TRP	6.4
1	A	157	ALA	6.3
1	A	269	CYS	6.2
1	A	254	THR	6.2
1	A	280	PHE	6.1
1	A	262	TRP	6.0
1	A	283	ILE	6.0
1	A	307	ARG	5.9
1	A	250	ALA	5.7
1	A	314	THR	5.7
1	A	268	VAL	5.6
1	A	272	ALA	5.6
1	A	276	PRO	5.6
1	A	222	TYR	5.5
1	A	275	THR	5.5
1	A	309	VAL	5.5
1	A	258	PRO	5.3
1	A	323	ALA	5.3
1	A	305	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	282	VAL	5.1
1	A	308	PRO	5.1
1	A	4	ASP	5.0
1	A	301	LEU	4.9
1	A	217	CYS	4.8
1	A	322	PHE	4.8
1	A	329	THR	4.7
1	A	315	SER	4.7
1	A	240	VAL	4.6
1	A	264	GLY	4.6
1	A	241	PHE	4.6
1	A	73	GLN	4.6
1	A	72	THR	4.5
1	A	384	TYR	4.5
1	A	311	ASP	4.5
1	A	328	SER	4.5
1	A	236	LEU	4.5
1	A	317	ASP	4.4
1	A	0	VAL	4.4
1	A	244	ALA	4.3
1	A	208	ILE	4.3
1	A	302	PRO	4.2
1	A	70	PRO	4.1
1	A	156	GLY	4.0
1	A	310	GLU	4.0
1	A	210	GLY	4.0
1	A	267	LEU	4.0
1	A	263	LEU	4.0
1	A	361	VAL	3.9
1	A	215	MET	3.9
1	A	233	ASN	3.9
1	A	367	THR	3.8
1	A	320	TYR	3.8
1	A	-1	PHE	3.8
1	A	306	LEU	3.7
1	A	68	TYR	3.7
1	A	69	VAL	3.7
1	A	168	ALA	3.6
1	A	359	CYS	3.6
1	A	273	GLY	3.6
1	A	300	ILE	3.6
1	A	332	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	212	ASP	3.5
1	A	331	THR	3.5
1	A	259	ASP	3.5
1	A	256	LYS	3.5
1	A	261	PHE	3.4
1	A	318	ASP	3.4
1	A	274	THR	3.4
1	A	381	ASP	3.4
1	A	211	GLN	3.4
1	A	74	GLY	3.4
1	A	255	GLU	3.3
1	A	243	ALA	3.3
1	A	251	ALA	3.3
1	A	237	PRO	3.3
1	A	67	VAL	3.3
1	A	213	LEU	3.3
1	A	281	PRO	3.3
1	A	316	GLN	3.3
1	A	363	ASP	3.3
1	A	324	ILE	3.2
1	A	386	ILE	3.2
1	A	248	ILE	3.2
1	A	253	SER	3.2
1	A	252	SER	3.2
1	A	260	GLY	3.1
1	A	231	THR	3.1
1	A	214	LYS	3.1
1	A	224	LYS	3.1
1	A	271	GLN	3.1
1	A	209	ASN	3.0
1	A	330	GLY	3.0
1	A	383	GLY	3.0
1	A	71	TYR	3.0
1	A	220	TYR	3.0
1	A	265	GLU	2.9
1	A	364	GLU	2.9
1	A	181	HIS	2.9
1	A	30	LEU	2.9
1	A	228	ASP	2.9
1	A	326	GLN	2.9
1	A	239	LYS	2.9
1	A	242	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	325	SER	2.8
1	A	327	SER	2.8
1	A	235	ARG	2.8
1	A	226	ILE	2.8
1	A	223	ASP	2.7
1	A	155	CYS	2.6
1	A	360	HIS	2.5
1	A	128	ARG	2.5
1	A	234	LEU	2.5
1	A	197	TRP	2.5
1	A	232	THR	2.5
1	A	336	VAL	2.4
1	A	219	GLU	2.3
1	A	382	CYS	2.3
1	A	385	ASN	2.3
1	A	216	ASP	2.3
1	A	238	LYS	2.3
1	A	169	SER	2.3
1	A	145	HIS	2.2
1	A	127	ALA	2.2
1	A	218	LYS	2.2
1	A	138	ASP	2.1
1	A	362	HIS	2.1
1	A	154	LEU	2.1
1	A	126	ILE	2.1
1	A	304	GLN	2.1
1	A	249	LYS	2.1
1	A	124	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOD	A	1504	1/1	0.90	0.30	54,54,54,54	1
2	IOD	A	1505	1/1	0.95	0.09	56,56,56,56	1
2	IOD	A	1503	1/1	0.98	0.10	35,35,35,35	1
2	IOD	A	1502	1/1	1.00	0.03	23,23,23,23	1

6.5 Other polymers [i](#)

There are no such residues in this entry.