



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:32 PM EDT

PDB ID : 1AOV
Title : APO DUCK OVOTRANSFERRIN
Authors : Rawas, A.; Muirhead, H.
Deposited on : 1996-12-11
Resolution : 4.00 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 : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

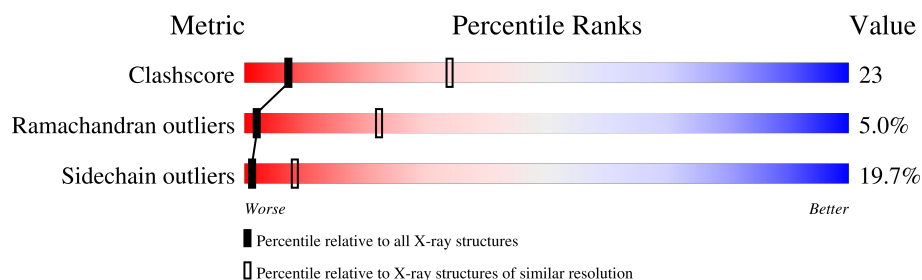
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)

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	686	<div> <div style="width: 44%; background-color: green;"></div> <div style="width: 39%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 4%; background-color: red;"></div> <div style="width: 4%; background-color: grey;"></div> </div> <div>44% 39% 13% .</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5299 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 APO-OVOTRANSFERRIN.

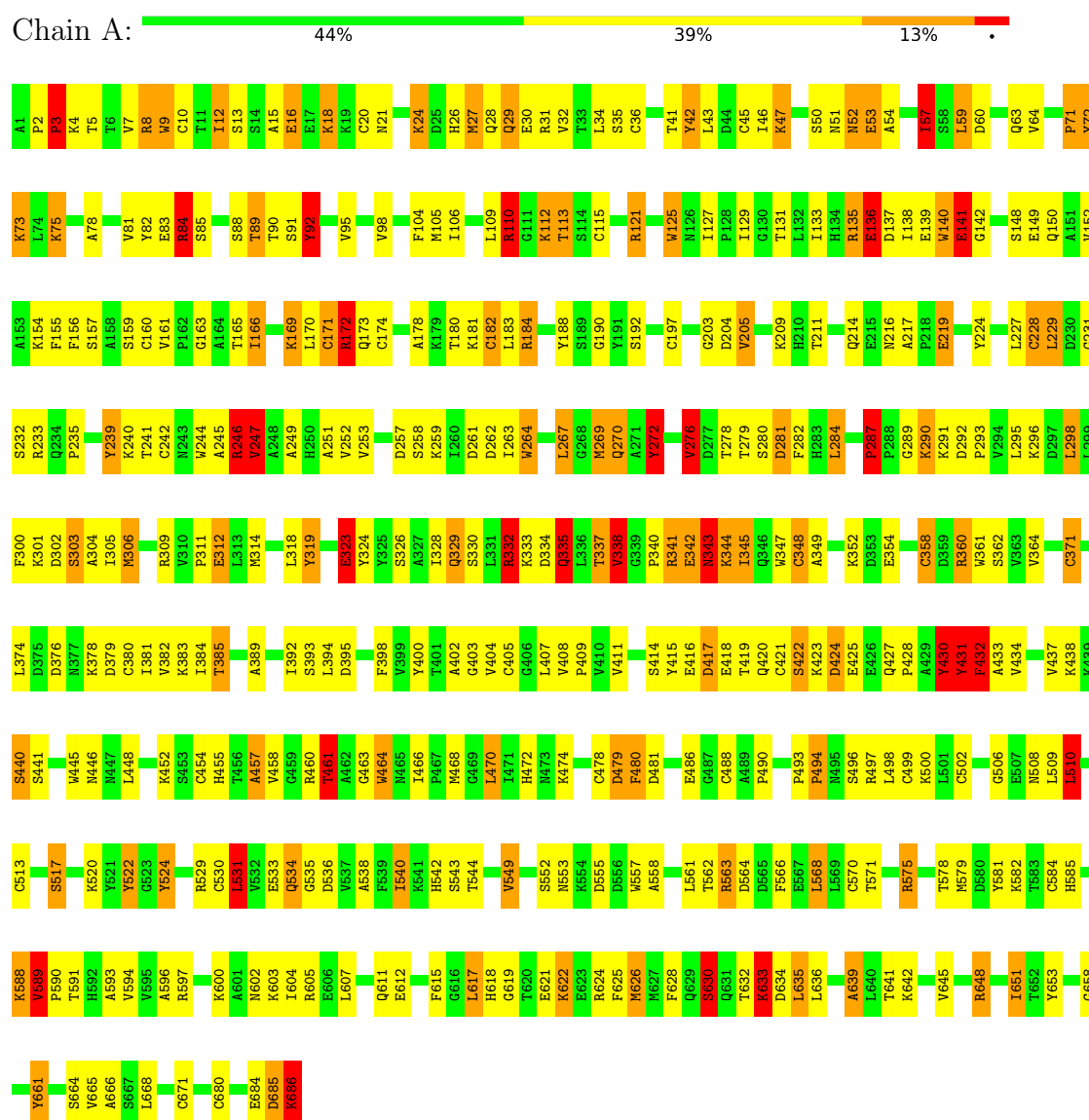
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	686	5299	3325	903	1032	39	0	0	0

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: APO-OVOTRANSFERRIN



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 21	Depositor
Cell constants a, b, c, α , β , γ	77.62Å 98.74Å 126.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 4.00	Depositor
% Data completeness (in resolution range)	92.8 (10.00-4.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.210 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5299	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	0.95	2/5397 (0.0%)	1.86	144/7277 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	TRP	CG-CD2	-5.45	1.34	1.43
1	A	464	TRP	CD1-NE1	-5.16	1.29	1.38

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	TYR	CB-CG-CD2	-14.77	112.14	121.00
1	A	432	PHE	CA-CB-CG	-10.81	87.96	113.90
1	A	82	TYR	CB-CG-CD2	-10.47	114.72	121.00
1	A	341	ARG	NE-CZ-NH1	10.35	125.48	120.30
1	A	140	TRP	CD1-CG-CD2	9.75	114.10	106.30
1	A	110	ARG	NE-CZ-NH1	9.23	124.91	120.30
1	A	335	GLN	CA-CB-CG	9.02	133.24	113.40
1	A	140	TRP	CE2-CD2-CG	-8.95	100.14	107.30
1	A	140	TRP	N-CA-CB	-8.86	94.66	110.60
1	A	341	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	281	ASP	N-CA-C	8.51	133.97	111.00
1	A	125	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	A	430	TYR	CA-CB-CG	8.45	129.45	113.40
1	A	92	TYR	N-CA-C	-8.40	88.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	361	TRP	CE2-CD2-CG	-8.14	100.79	107.30
1	A	685	ASP	N-CA-C	-8.02	89.36	111.00
1	A	224	TYR	CB-CG-CD1	-7.99	116.20	121.00
1	A	588	LYS	CA-CB-CG	-7.97	95.87	113.40
1	A	125	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	A	9	TRP	CE2-CD2-CG	-7.93	100.95	107.30
1	A	557	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	84	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	A	92	TYR	CB-CG-CD2	-7.73	116.36	121.00
1	A	247	VAL	N-CA-C	-7.62	90.44	111.00
1	A	648	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	588	LYS	N-CA-C	7.55	131.37	111.00
1	A	337	THR	N-CA-C	7.45	131.11	111.00
1	A	445	TRP	CD1-CG-CD2	7.32	112.16	106.30
1	A	334	ASP	CA-C-N	-7.28	101.19	117.20
1	A	140	TRP	CB-CG-CD1	-7.25	117.57	127.00
1	A	557	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	A	184	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	358	CYS	CA-CB-SG	-7.24	100.97	114.00
1	A	9	TRP	CD1-CG-CD2	7.21	112.06	106.30
1	A	633	LYS	CA-CB-CG	7.16	129.16	113.40
1	A	361	TRP	CD1-CG-CD2	7.16	112.03	106.30
1	A	686	LYS	CA-CB-CG	7.15	129.12	113.40
1	A	110	ARG	CA-C-N	-7.15	101.91	116.20
1	A	244	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	A	464	TRP	CD1-CG-CD2	7.01	111.91	106.30
1	A	445	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	A	361	TRP	CG-CD2-CE3	6.98	140.18	133.90
1	A	135	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	52	ASN	N-CA-CB	-6.95	98.08	110.60
1	A	680	CYS	CA-CB-SG	-6.92	101.54	114.00
1	A	323	GLU	N-CA-CB	-6.91	98.16	110.60
1	A	73	LYS	CA-CB-CG	6.90	128.57	113.40
1	A	110	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	464	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	A	306	MET	CA-CB-CG	6.87	124.99	113.30
1	A	148	SER	N-CA-CB	-6.87	100.20	110.50
1	A	91	SER	C-N-CA	6.79	138.68	121.70
1	A	169	LYS	CB-CG-CD	-6.75	94.05	111.60
1	A	270	GLN	CA-CB-CG	6.70	128.15	113.40
1	A	348	CYS	CA-CB-SG	-6.66	102.01	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	GLU	CA-C-N	-6.59	102.69	117.20
1	A	16	GLU	CA-CB-CG	-6.58	98.92	113.40
1	A	246	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	A	264	TRP	CD1-CG-CD2	6.56	111.55	106.30
1	A	264	TRP	CE2-CD2-CG	-6.55	102.06	107.30
1	A	468	MET	CG-SD-CE	6.52	110.63	100.20
1	A	431	TYR	CA-C-N	6.43	131.34	117.20
1	A	581	TYR	N-CA-C	6.40	128.28	111.00
1	A	244	TRP	CG-CD2-CE3	6.38	139.64	133.90
1	A	247	VAL	CG1-CB-CG2	-6.36	100.72	110.90
1	A	83	GLU	N-CA-C	6.31	128.05	111.00
1	A	431	TYR	CA-CB-CG	6.27	125.31	113.40
1	A	524	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	171	CYS	CA-CB-SG	6.21	125.18	114.00
1	A	84	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	431	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	A	141	GLU	N-CA-C	6.07	127.37	111.00
1	A	51	ASN	N-CA-C	-6.02	94.73	111.00
1	A	445	TRP	CB-CG-CD1	-6.01	119.19	127.00
1	A	9	TRP	CG-CD2-CE3	6.00	139.29	133.90
1	A	73	LYS	N-CA-C	-5.95	94.94	111.00
1	A	140	TRP	CA-C-N	5.94	130.26	117.20
1	A	82	TYR	N-CA-C	5.92	126.98	111.00
1	A	589	VAL	CA-CB-CG2	-5.90	102.04	110.90
1	A	136	GLU	CA-CB-CG	5.90	126.39	113.40
1	A	57	ILE	CB-CA-C	-5.89	99.81	111.60
1	A	84	ARG	CA-CB-CG	5.89	126.35	113.40
1	A	3	PRO	CA-N-CD	-5.88	103.27	111.50
1	A	8	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	497	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	140	TRP	CG-CD2-CE3	5.87	139.18	133.90
1	A	347	TRP	CE2-CD2-CG	-5.85	102.62	107.30
1	A	497	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	557	TRP	CG-CD2-CE3	5.77	139.09	133.90
1	A	557	TRP	CB-CG-CD1	-5.77	119.50	127.00
1	A	140	TRP	CB-CA-C	5.73	121.86	110.40
1	A	140	TRP	CG-CD1-NE1	-5.73	104.37	110.10
1	A	347	TRP	CD1-CG-CD2	5.72	110.87	106.30
1	A	91	SER	CA-C-N	-5.66	104.74	117.20
1	A	276	VAL	CA-CB-CG1	-5.66	102.41	110.90
1	A	345	ILE	N-CA-C	-5.64	95.78	111.00
1	A	182	CYS	CA-CB-SG	-5.63	103.87	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	TYR	CA-C-O	-5.61	108.31	120.10
1	A	287	PRO	N-CA-C	5.61	126.69	112.10
1	A	575	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	630	SER	N-CA-CB	-5.55	102.18	110.50
1	A	605	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	338	VAL	CA-CB-CG1	-5.53	102.60	110.90
1	A	635	LEU	N-CA-C	-5.53	96.06	111.00
1	A	304	ALA	CA-C-N	-5.49	105.11	117.20
1	A	334	ASP	O-C-N	5.48	131.47	122.70
1	A	480	PHE	CA-CB-CG	-5.48	100.75	113.90
1	A	352	LYS	CA-CB-CG	5.46	125.41	113.40
1	A	332	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	653	TYR	CA-CB-CG	5.45	123.75	113.40
1	A	53	GLU	CB-CA-C	-5.44	99.51	110.40
1	A	290	LYS	CA-C-N	-5.38	105.36	117.20
1	A	634	ASP	N-CA-C	-5.38	96.48	111.00
1	A	344	LYS	N-CA-CB	5.36	120.25	110.60
1	A	31	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	622	LYS	CA-CB-CG	5.35	125.18	113.40
1	A	648	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	148	SER	N-CA-C	5.29	125.29	111.00
1	A	423	LYS	N-CA-C	-5.28	96.75	111.00
1	A	563	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	125	TRP	CB-CG-CD1	-5.21	120.22	127.00
1	A	684	GLU	CA-C-N	-5.20	105.76	117.20
1	A	172	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	29	GLN	CA-C-N	5.19	128.61	117.20
1	A	589	VAL	N-CA-CB	-5.18	100.10	111.50
1	A	278	THR	N-CA-C	-5.17	97.03	111.00
1	A	161	VAL	N-CA-C	-5.16	97.06	111.00
1	A	121	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	531	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	235	PRO	CA-C-N	-5.15	105.87	117.20
1	A	272	TYR	CG-CD2-CE2	-5.15	117.18	121.30
1	A	522	TYR	CB-CG-CD1	-5.14	117.91	121.00
1	A	188	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	634	ASP	CA-C-N	-5.13	105.92	117.20
1	A	510	LEU	N-CA-C	5.10	124.78	111.00
1	A	474	LYS	CB-CG-CD	-5.10	98.34	111.60
1	A	269	MET	CG-SD-CE	-5.10	92.05	100.20
1	A	335	GLN	CG-CD-NE2	5.07	128.86	116.70
1	A	414	SER	CA-C-N	-5.05	106.09	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASN	CB-CA-C	5.04	120.49	110.40
1	A	593	ALA	CA-C-N	5.03	128.27	117.20
1	A	319	TYR	CB-CG-CD2	-5.00	118.00	121.00
1	A	445	TRP	CG-CD2-CE3	5.00	138.40	133.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	TYR	Sidechain
1	A	42	TYR	Sidechain
1	A	431	TYR	Sidechain
1	A	432	PHE	Sidechain

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	5299	0	5218	227	0
All	All	5299	0	5218	227	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 23.

All (227) 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:454:CYS:HG	1:A:530:CYS:HG	1.01	0.91
1:A:394:LEU:HD13	1:A:398:PHE:HB3	1.51	0.89
1:A:358:CYS:SG	1:A:371:CYS:HB3	2.14	0.87
1:A:228:CYS:HG	1:A:242:CYS:HG	1.10	0.86
1:A:430:TYR:HB3	1:A:590:PRO:HA	1.58	0.85
1:A:246:ARG:NH2	1:A:686:LYS:HB2	1.92	0.84
1:A:478:CYS:HG	1:A:671:CYS:HG	0.89	0.82
1:A:20:CYS:HG	1:A:36:CYS:HG	1.02	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG11	1:A:263:ILE:HG23	1.64	0.80
1:A:454:CYS:SG	1:A:535:GLY:HA3	2.23	0.78
1:A:437:VAL:HA	1:A:531:LEU:HD21	1.67	0.76
1:A:115:CYS:SG	1:A:203:GLY:HA3	2.26	0.75
1:A:81:VAL:HB	1:A:306:MET:HB3	1.68	0.75
1:A:140:TRP:H	1:A:337:THR:HG21	1.51	0.74
1:A:457:ALA:HB3	1:A:460:ARG:HD3	1.68	0.74
1:A:141:GLU:HA	1:A:335:GLN:HB3	1.69	0.74
1:A:163:GLY:HA3	1:A:184:ARG:HG2	1.71	0.73
1:A:98:VAL:HG11	1:A:227:LEU:HD13	1.71	0.72
1:A:9:TRP:HB2	1:A:34:LEU:HD11	1.70	0.72
1:A:26:HIS:CE1	1:A:282:PHE:HB2	2.26	0.70
1:A:10:CYS:HB3	1:A:57:ILE:HG23	1.75	0.69
1:A:135:ARG:HA	1:A:340:PRO:HB3	1.74	0.68
1:A:209:LYS:HE2	1:A:211:THR:OG1	1.95	0.67
1:A:127:ILE:HD12	1:A:245:ALA:HB3	1.75	0.67
1:A:228:CYS:CB	1:A:242:CYS:SG	2.83	0.67
1:A:228:CYS:HB3	1:A:242:CYS:SG	2.35	0.67
1:A:434:VAL:HG21	1:A:568:LEU:HG	1.77	0.67
1:A:140:TRP:CE2	1:A:335:GLN:HG2	2.30	0.66
1:A:228:CYS:CB	1:A:242:CYS:HG	2.08	0.66
1:A:15:ALA:O	1:A:18:LYS:HB3	1.96	0.65
1:A:343:ASN:ND2	1:A:343:ASN:H	1.95	0.65
1:A:59:LEU:HG	1:A:63:GLN:HB3	1.79	0.65
1:A:140:TRP:CE3	1:A:335:GLN:HA	2.32	0.64
1:A:452:LYS:HA	1:A:486:GLU:O	1.98	0.64
1:A:267:LEU:HA	1:A:270:GLN:HG3	1.78	0.64
1:A:329:GLN:HE21	1:A:329:GLN:HA	1.61	0.64
1:A:105:MET:SD	1:A:233:ARG:HG3	2.38	0.63
1:A:382:VAL:HA	1:A:385:THR:OG1	1.99	0.63
1:A:115:CYS:CB	1:A:197:CYS:HG	2.12	0.62
1:A:150:GLN:HE21	1:A:166:ILE:HG13	1.64	0.62
1:A:432:PHE:HB3	1:A:433:ALA:N	2.13	0.62
1:A:113:THR:OG1	1:A:203:GLY:HA2	1.99	0.62
1:A:245:ALA:HB2	1:A:323:GLU:HB3	1.82	0.62
1:A:454:CYS:CB	1:A:530:CYS:HG	2.13	0.62
1:A:192:SER:HB3	1:A:216:ASN:HD21	1.65	0.61
1:A:106:ILE:HG22	1:A:231:GLY:HA2	1.82	0.61
1:A:421:CYS:H	1:A:424:ASP:HB3	1.65	0.61
1:A:420:GLN:HA	1:A:424:ASP:O	2.00	0.61
1:A:566:PHE:O	1:A:578:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD23	1:A:64:VAL:HA	1.83	0.61
1:A:409:PRO:HG2	1:A:651:ILE:HG23	1.83	0.59
1:A:47:LYS:HA	1:A:50:SER:OG	2.02	0.59
1:A:630:SER:HB3	1:A:635:LEU:HD12	1.85	0.59
1:A:437:VAL:HG12	1:A:536:ASP:O	2.04	0.58
1:A:106:ILE:HD13	1:A:229:LEU:HA	1.86	0.58
1:A:20:CYS:HG	1:A:36:CYS:CB	2.16	0.57
1:A:129:ILE:HD12	1:A:152:VAL:HG11	1.86	0.57
1:A:142:GLY:H	1:A:335:GLN:HB2	1.68	0.57
1:A:364:VAL:HG23	1:A:624:ARG:NH1	2.18	0.57
1:A:633:LYS:O	1:A:639:ALA:HB2	2.04	0.57
1:A:109:LEU:HD23	1:A:112:LYS:HG2	1.87	0.57
1:A:430:TYR:CE2	1:A:588:LYS:HG2	2.40	0.57
1:A:10:CYS:SG	1:A:45:CYS:HB3	2.44	0.56
1:A:400:TYR:O	1:A:404:VAL:HG23	2.05	0.56
1:A:626:MET:SD	1:A:628:PHE:HB2	2.45	0.56
1:A:140:TRP:HZ3	1:A:330:SER:O	1.88	0.56
1:A:374:LEU:HD11	1:A:383:LYS:HG3	1.87	0.56
1:A:499:CYS:CB	1:A:513:CYS:HG	2.18	0.56
1:A:81:VAL:HA	1:A:89:THR:O	2.05	0.56
1:A:21:ASN:HA	1:A:24:LYS:HG2	1.87	0.55
1:A:21:ASN:O	1:A:24:LYS:HG3	2.06	0.55
1:A:141:GLU:CA	1:A:335:GLN:HB3	2.35	0.55
1:A:590:PRO:HD2	1:A:661:TYR:HD2	1.71	0.55
1:A:43:LEU:O	1:A:46:ILE:HB	2.07	0.55
1:A:402:ALA:HB1	1:A:407:LEU:HD12	1.87	0.55
1:A:600:LYS:O	1:A:604:ILE:HG13	2.07	0.55
1:A:75:LYS:HE3	1:A:314:MET:O	2.06	0.55
1:A:618:HIS:HA	1:A:622:LYS:NZ	2.22	0.55
1:A:457:ALA:HA	1:A:490:PRO:HD2	1.90	0.54
1:A:324:TYR:CE1	1:A:328:ILE:HD11	2.43	0.54
1:A:524:TYR:HA	1:A:540:ILE:HD11	1.90	0.54
1:A:328:ILE:O	1:A:332:ARG:HB3	2.08	0.54
1:A:392:ILE:HG12	1:A:393:SER:N	2.22	0.53
1:A:251:ALA:HB2	1:A:319:TYR:HE2	1.73	0.53
1:A:324:TYR:CZ	1:A:328:ILE:HD11	2.44	0.53
1:A:60:ASP:O	1:A:64:VAL:HG12	2.08	0.53
1:A:292:ASP:O	1:A:295:LEU:HB2	2.10	0.52
1:A:472:HIS:CE1	1:A:671:CYS:SG	3.03	0.52
1:A:57:ILE:HD12	1:A:59:LEU:HD13	1.90	0.52
1:A:180:THR:HA	1:A:183:LEU:HG	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:CYS:O	1:A:174:CYS:SG	2.68	0.52
1:A:267:LEU:O	1:A:270:GLN:HG3	2.10	0.52
1:A:428:PRO:HD3	1:A:645:VAL:HG11	1.91	0.51
1:A:493:PRO:HG2	1:A:496:SER:HB2	1.92	0.51
1:A:590:PRO:HD2	1:A:661:TYR:CD2	2.45	0.51
1:A:420:GLN:HB3	1:A:425:GLU:HA	1.93	0.51
1:A:142:GLY:H	1:A:335:GLN:CB	2.23	0.51
1:A:570:CYS:CB	1:A:584:CYS:HG	2.21	0.51
1:A:59:LEU:HG	1:A:63:GLN:CB	2.41	0.51
1:A:42:TYR:HA	1:A:45:CYS:SG	2.51	0.51
1:A:438:LYS:HG3	1:A:531:LEU:HD22	1.93	0.51
1:A:282:PHE:CE2	1:A:284:LEU:HD22	2.47	0.50
1:A:282:PHE:HE2	1:A:284:LEU:HD22	1.77	0.50
1:A:488:CYS:CB	1:A:502:CYS:HG	2.24	0.50
1:A:160:CYS:HB2	1:A:173:GLN:HB2	1.93	0.50
1:A:171:CYS:C	1:A:174:CYS:HG	2.15	0.50
1:A:264:TRP:CZ2	1:A:309:ARG:HB2	2.47	0.50
1:A:494:PRO:HA	1:A:499:CYS:SG	2.51	0.50
1:A:110:ARG:HG3	1:A:110:ARG:HH11	1.76	0.49
1:A:343:ASN:H	1:A:343:ASN:HD22	1.58	0.49
1:A:422:SER:O	1:A:425:GLU:HG2	2.12	0.49
1:A:5:THR:O	1:A:32:VAL:HA	2.13	0.49
1:A:10:CYS:SG	1:A:45:CYS:SG	3.10	0.49
1:A:392:ILE:HG23	1:A:394:LEU:HG	1.95	0.49
1:A:568:LEU:CD1	1:A:578:THR:HA	2.43	0.49
1:A:607:LEU:O	1:A:611:GLN:HG2	2.12	0.49
1:A:10:CYS:HG	1:A:45:CYS:HB3	1.77	0.49
1:A:291:LYS:HD3	1:A:296:LYS:HE3	1.94	0.49
1:A:432:PHE:CZ	1:A:582:LYS:HA	2.47	0.48
1:A:121:ARG:CZ	1:A:190:GLY:HA2	2.44	0.48
1:A:524:TYR:HD1	1:A:540:ILE:HG13	1.78	0.48
1:A:457:ALA:HB2	1:A:522:TYR:HE1	1.78	0.48
1:A:174:CYS:HB2	1:A:181:LYS:HD2	1.94	0.48
1:A:121:ARG:NH2	1:A:190:GLY:HA2	2.28	0.48
1:A:104:PHE:CZ	1:A:204:ASP:HB3	2.48	0.48
1:A:142:GLY:N	1:A:335:GLN:HB2	2.29	0.48
1:A:520:LYS:HE2	1:A:529:ARG:NH2	2.29	0.48
1:A:12:ILE:HG22	1:A:45:CYS:SG	2.54	0.48
1:A:16:GLU:OE2	1:A:298:LEU:HA	2.13	0.48
1:A:159:SER:HB2	1:A:170:LEU:HA	1.94	0.48
1:A:98:VAL:HG12	1:A:205:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:H	1:A:166:ILE:HD13	1.79	0.47
1:A:292:ASP:H	1:A:295:LEU:HD12	1.79	0.47
1:A:488:CYS:CB	1:A:502:CYS:SG	3.02	0.47
1:A:104:PHE:H	1:A:233:ARG:NH2	2.11	0.47
1:A:380:CYS:O	1:A:384:ILE:HG13	2.14	0.47
1:A:403:GLY:HA2	1:A:407:LEU:O	2.14	0.47
1:A:284:LEU:HD12	1:A:300:PHE:HD2	1.79	0.47
1:A:360:ARG:HH11	1:A:625:PHE:HB2	1.79	0.47
1:A:531:LEU:HG	1:A:538:ALA:HB2	1.96	0.47
1:A:341:ARG:O	1:A:343:ASN:N	2.47	0.47
1:A:348:CYS:HB2	1:A:389:ALA:HB1	1.96	0.47
1:A:125:TRP:O	1:A:129:ILE:HB	2.15	0.47
1:A:393:SER:HA	1:A:594:VAL:HG12	1.97	0.47
1:A:138:ILE:HG12	1:A:155:PHE:CG	2.49	0.47
1:A:92:TYR:O	1:A:247:VAL:N	2.49	0.46
1:A:455:HIS:HD2	1:A:463:GLY:O	1.99	0.46
1:A:481:ASP:HA	1:A:498:LEU:HD11	1.98	0.46
1:A:169:LYS:HG2	1:A:172:ARG:NH1	2.31	0.46
1:A:269:MET:HA	1:A:272:TYR:HE1	1.81	0.46
1:A:276:VAL:HG11	1:A:305:ILE:HG22	1.97	0.46
1:A:506:GLY:HA2	1:A:520:LYS:HE3	1.97	0.46
1:A:78:ALA:HB3	1:A:252:VAL:HB	1.98	0.46
1:A:454:CYS:HB3	1:A:530:CYS:SG	2.56	0.46
1:A:466:ILE:O	1:A:470:LEU:HD22	2.16	0.46
1:A:3:PRO:HG3	1:A:262:ASP:OD1	2.16	0.46
1:A:59:LEU:HB3	1:A:64:VAL:HB	1.98	0.46
1:A:142:GLY:N	1:A:335:GLN:CB	2.79	0.46
1:A:84:ARG:HG2	1:A:85:SER:H	1.81	0.45
1:A:246:ARG:CZ	1:A:686:LYS:HB2	2.45	0.45
1:A:461:THR:CG2	1:A:589:VAL:HG21	2.46	0.45
1:A:329:GLN:HA	1:A:329:GLN:NE2	2.29	0.45
1:A:272:TYR:CD1	1:A:272:TYR:N	2.84	0.45
1:A:341:ARG:O	1:A:603:LYS:HE2	2.17	0.45
1:A:8:ARG:HB2	1:A:54:ALA:HA	1.99	0.45
1:A:589:VAL:HG22	1:A:661:TYR:CE2	2.52	0.45
1:A:295:LEU:O	1:A:298:LEU:HD22	2.17	0.45
1:A:8:ARG:HA	1:A:35:SER:HB3	1.99	0.44
1:A:301:LYS:HB3	1:A:303:SER:OG	2.18	0.44
1:A:157:SER:O	1:A:169:LYS:HD3	2.17	0.44
1:A:381:ILE:HG23	1:A:407:LEU:HD11	1.98	0.44
1:A:533:GLU:HB3	1:A:534:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:HD2	1:A:156:PHE:CD2	2.35	0.44
1:A:415:TYR:HD1	1:A:641:THR:HA	1.82	0.44
1:A:420:GLN:HA	1:A:425:GLU:HA	1.99	0.44
1:A:597:ARG:HE	1:A:597:ARG:HB3	1.69	0.44
1:A:344:LYS:O	1:A:345:ILE:N	2.50	0.44
1:A:615:PHE:CE1	1:A:621:GLU:HB2	2.53	0.44
1:A:131:THR:HG22	1:A:135:ARG:HD2	1.99	0.44
1:A:71:PRO:HD2	1:A:72:TYR:CE1	2.53	0.43
1:A:136:GLU:O	1:A:139:GLU:HG3	2.18	0.43
1:A:420:GLN:HG2	1:A:427:GLN:O	2.18	0.43
1:A:481:ASP:HA	1:A:498:LEU:CD1	2.49	0.43
1:A:81:VAL:HG13	1:A:89:THR:H	1.84	0.43
1:A:267:LEU:CA	1:A:270:GLN:HG3	2.45	0.43
1:A:479:ASP:O	1:A:481:ASP:N	2.52	0.43
1:A:358:CYS:HG	1:A:371:CYS:HB3	1.81	0.43
1:A:619:GLY:H	1:A:622:LYS:HD3	1.83	0.43
1:A:135:ARG:O	1:A:340:PRO:HD3	2.18	0.43
1:A:349:ALA:HB1	1:A:354:GLU:HB3	2.00	0.43
1:A:407:LEU:HA	1:A:596:ALA:O	2.19	0.42
1:A:457:ALA:HB3	1:A:460:ARG:CD	2.44	0.42
1:A:71:PRO:HD2	1:A:72:TYR:CZ	2.53	0.42
1:A:408:VAL:HA	1:A:409:PRO:HD2	1.87	0.42
1:A:416:GLU:HB2	1:A:419:THR:OG1	2.19	0.42
1:A:417:ASP:HB3	1:A:642:LYS:HD2	2.01	0.42
1:A:540:ILE:HG12	1:A:544:THR:OG1	2.20	0.42
1:A:42:TYR:O	1:A:46:ILE:HG13	2.20	0.42
1:A:7:VAL:O	1:A:35:SER:N	2.52	0.42
1:A:110:ARG:HG2	1:A:155:PHE:CE1	2.54	0.42
1:A:420:GLN:CA	1:A:425:GLU:HA	2.50	0.42
1:A:314:MET:SD	1:A:318:LEU:HB2	2.59	0.42
1:A:329:GLN:O	1:A:333:LYS:HB2	2.19	0.42
1:A:438:LYS:HG2	1:A:566:PHE:HE1	1.85	0.42
1:A:287:PRO:HB3	1:A:302:ASP:HB3	2.02	0.42
1:A:432:PHE:CE2	1:A:585:HIS:ND1	2.88	0.41
1:A:10:CYS:HG	1:A:45:CYS:CB	2.32	0.41
1:A:217:ALA:O	1:A:219:GLU:N	2.54	0.41
1:A:376:ASP:HB2	1:A:379:ASP:H	1.85	0.41
1:A:589:VAL:HA	1:A:590:PRO:HD2	1.98	0.41
1:A:81:VAL:HG11	1:A:88:SER:HB2	2.02	0.41
1:A:133:ILE:HG21	1:A:330:SER:HB3	2.02	0.41
1:A:668:LEU:O	1:A:671:CYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TYR:CZ	1:A:240:LYS:HE3	2.56	0.41
1:A:305:ILE:HD13	1:A:305:ILE:HG21	1.89	0.41
1:A:582:LYS:O	1:A:585:HIS:CE1	2.74	0.41
1:A:582:LYS:O	1:A:585:HIS:HE1	2.04	0.41
1:A:135:ARG:O	1:A:136:GLU:HB3	2.22	0.40
1:A:440:SER:O	1:A:575:ARG:NH2	2.55	0.40
1:A:458:VAL:HG13	1:A:464:TRP:CE2	2.56	0.40
1:A:665:VAL:HG13	1:A:666:ALA:N	2.35	0.40
1:A:282:PHE:HE2	1:A:284:LEU:CD2	2.35	0.40
1:A:416:GLU:C	1:A:418:GLU:H	2.25	0.40
1:A:630:SER:HB2	1:A:632:THR:O	2.22	0.40
1:A:27:MET:N	1:A:27:MET:SD	2.94	0.40
1:A:420:GLN:CB	1:A:425:GLU:HA	2.52	0.40
1:A:558:ALA:HA	1:A:561:LEU:HD12	2.04	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	674/686 (98%)	555 (82%)	85 (13%)	34 (5%)	2	22

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	136	GLU
1	A	249	ALA
1	A	289	GLY
1	A	290	LYS
1	A	312	GLU
1	A	342	GLU

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Mol	Chain	Res	Type
1	A	343	ASN
1	A	440	SER
1	A	480	PHE
1	A	510	LEU
1	A	685	ASP
1	A	259	LYS
1	A	323	GLU
1	A	430	TYR
1	A	509	LEU
1	A	579	MET
1	A	639	ALA
1	A	422	SER
1	A	461	THR
1	A	517	SER
1	A	29	GLN
1	A	178	ALA
1	A	457	ALA
1	A	591	THR
1	A	617	LEU
1	A	636	LEU
1	A	311	PRO
1	A	417	ASP
1	A	137	ASP
1	A	335	GLN
1	A	549	VAL
1	A	658	GLY
1	A	338	VAL

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	578/578 (100%)	464 (80%)	114 (20%)	1 8

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	3	PRO
1	A	4	LYS
1	A	12	ILE
1	A	13	SER
1	A	18	LYS
1	A	24	LYS
1	A	27	MET
1	A	28	GLN
1	A	30	GLU
1	A	41	THR
1	A	47	LYS
1	A	52	ASN
1	A	53	GLU
1	A	57	ILE
1	A	59	LEU
1	A	71	PRO
1	A	72	TYR
1	A	73	LYS
1	A	75	LYS
1	A	84	ARG
1	A	89	THR
1	A	90	THR
1	A	92	TYR
1	A	95	VAL
1	A	110	ARG
1	A	112	LYS
1	A	113	THR
1	A	136	GLU
1	A	141	GLU
1	A	149	GLU
1	A	154	LYS
1	A	166	ILE
1	A	172	ARG
1	A	182	CYS
1	A	205	VAL
1	A	214	GLN
1	A	219	GLU
1	A	228	CYS
1	A	229	LEU
1	A	232	SER
1	A	239	TYR
1	A	241	THR

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Mol	Chain	Res	Type
1	A	246	ARG
1	A	247	VAL
1	A	253	VAL
1	A	257	ASP
1	A	258	SER
1	A	261	ASP
1	A	267	LEU
1	A	276	VAL
1	A	279	THR
1	A	280	SER
1	A	281	ASP
1	A	284	LEU
1	A	287	PRO
1	A	293	PRO
1	A	298	LEU
1	A	303	SER
1	A	312	GLU
1	A	326	SER
1	A	329	GLN
1	A	332	ARG
1	A	338	VAL
1	A	343	ASN
1	A	360	ARG
1	A	362	SER
1	A	371	CYS
1	A	378	LYS
1	A	385	THR
1	A	395	ASP
1	A	405	CYS
1	A	411	VAL
1	A	424	ASP
1	A	430	TYR
1	A	431	TYR
1	A	432	PHE
1	A	441	SER
1	A	446	ASN
1	A	448	LEU
1	A	461	THR
1	A	470	LEU
1	A	479	ASP
1	A	494	PRO
1	A	500	LYS

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Mol	Chain	Res	Type
1	A	508	ASN
1	A	510	LEU
1	A	517	SER
1	A	531	LEU
1	A	534	GLN
1	A	540	ILE
1	A	542	HIS
1	A	543	SER
1	A	549	VAL
1	A	552	SER
1	A	553	ASN
1	A	555	ASP
1	A	562	THR
1	A	563	ARG
1	A	564	ASP
1	A	568	LEU
1	A	571	THR
1	A	589	VAL
1	A	602	ASN
1	A	612	GLU
1	A	617	LEU
1	A	626	MET
1	A	630	SER
1	A	633	LYS
1	A	648	ARG
1	A	651	ILE
1	A	661	TYR
1	A	664	SER
1	A	686	LYS

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

Mol	Chain	Res	Type
1	A	126	ASN
1	A	150	GLN
1	A	214	GLN
1	A	216	ASN
1	A	329	GLN
1	A	335	GLN
1	A	343	ASN
1	A	455	HIS
1	A	534	GLN

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Mol	Chain	Res	Type
1	A	553	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	245:ALA	C	246:ARG	N	4.94
1	A	587:ALA	C	588:LYS	N	3.36
1	A	432:PHE	C	433:ALA	N	3.21
1	A	92:TYR	C	93:TYR	N	3.19
1	A	344:LYS	C	345:ILE	N	2.88

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.