



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:15 PM GMT

PDB ID : 1JF6
Title : Crystal structure of thermoactinomyces vulgaris r-47 alpha-amylase mutant F286Y
Authors : Ohtaki, A.; Kondo, S.; Shimura, Y.; Tonozuka, T.; Sakano, Y.; Kamitori, S.
Deposited on : 2001-06-20
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

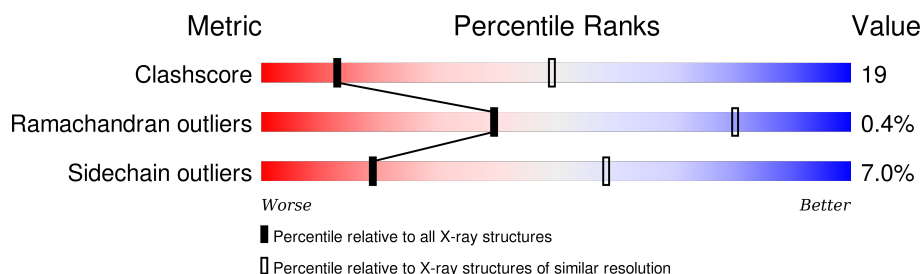
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	585	 58% 39% •
1	B	585	 59% 37% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9556 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 ALPHA AMYLASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4777	3056	831	875	15			
1	B	585	Total	C	N	O	S	0	0	0
			4777	3056	831	875	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	TYR	PHE	ENGINEERED	UNP Q08751
B	286	TYR	PHE	ENGINEERED	UNP Q08751

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

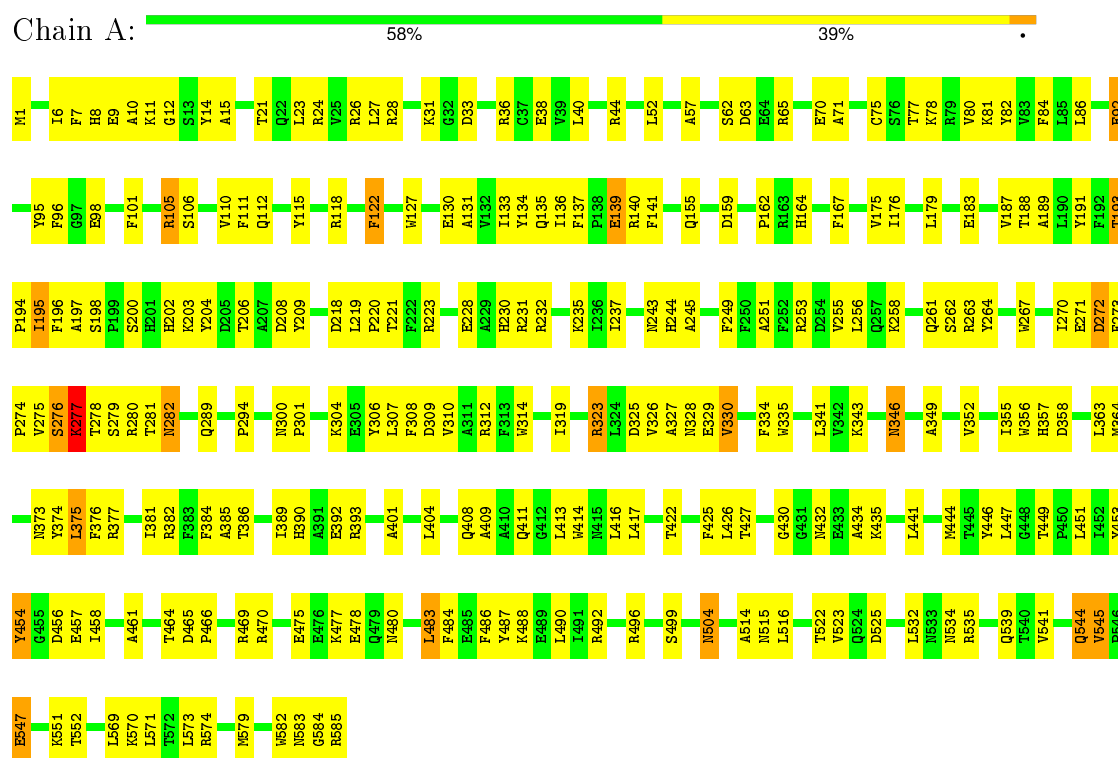
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

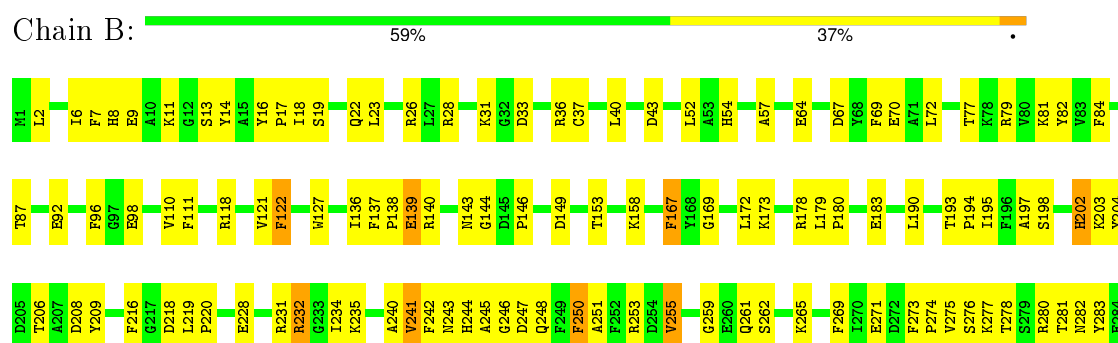
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ALPHA AMYLASE II



• Molecule 1: ALPHA AMYLASE II



R469	R470	P471	N472	K570	L571	T572	L573	Y576	M579	H580	L581	W582	N583	G584	R585																																	
Y374	L375	F376	R377	V380	I381	F384	A385	I389	H390	A391	E392	R393	L398	P406	Q411	W414	N415	L416		R424	F425	L426	T427	S428	F436	R437	L438	P442	L447	G448	T449	P450	L451	I452	Y453	Y454	G455	D456	E457	I458	G459	M460	A461	T464	D465	P466	D467	C468
T285	Y286	Q289	A292	N293	F294	K295	L296	R297	I300	F301	E302	D309	R312	M315	E316	Q317	G318	I319	W322	R323	L324	D325	I328	E329	V330	D331	H332	A333	F334	W335	R336	E337	F338	R339	R340	V352	G353	E354	I355	W356	H357	D358	W364	Q367	W371	W372	I373	

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 21	Depositor
Cell constants a, b, c, α , β , γ	112.25Å 117.94Å 113.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.39 – 3.20	Depositor
% Data completeness (in resolution range)	91.7 (38.39-3.20)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9556	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	0/4907	0.66	0/6643
1	B	0.50	0/4907	0.66	0/6643
All	All	0.50	0/9814	0.66	0/13286

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	TYR	Sidechain

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	4777	0	4607	184	0
1	B	4777	0	4607	181	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	9556	0	9214	361	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (361) 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:328:ASN:HB3	1:A:355:ILE:HD12	1.40	1.02
1:A:255:VAL:HA	1:A:262:SER:OG	1.67	0.93
1:A:162:PRO:HG2	1:A:470:ARG:HA	1.60	0.83
1:B:26:ARG:HG2	1:B:70:GLU:HG2	1.62	0.81
1:A:197:ALA:HB3	1:A:208:ASP:HB3	1.62	0.79
1:A:416:LEU:HD23	1:A:416:LEU:H	1.47	0.79
1:B:328:ASN:HB3	1:B:355:ILE:HG12	1.67	0.76
1:B:499:SER:HB3	1:B:523:VAL:HG12	1.67	0.75
1:B:247:ASP:HB3	1:B:292:ALA:HA	1.69	0.73
1:B:255:VAL:O	1:B:275:VAL:HG21	1.89	0.72
1:B:569:LEU:HD23	1:B:571:LEU:HD21	1.69	0.72
1:A:401:ALA:O	1:A:404:LEU:HB2	1.90	0.72
1:B:26:ARG:HG2	1:B:70:GLU:CG	2.21	0.70
1:B:138:PRO:HG3	1:B:195:ILE:HG22	1.73	0.70
1:A:582:TRP:CZ2	1:A:584:GLY:HA2	2.27	0.70
1:A:275:VAL:O	1:A:276:SER:HB2	1.91	0.69
1:A:133:ILE:HG13	1:A:189:ALA:HB3	1.76	0.68
1:A:514:ALA:HB1	1:A:539:GLN:HE22	1.59	0.68
1:A:98:GLU:OE2	1:B:357:HIS:HB2	1.94	0.67
1:B:202:HIS:CD2	1:B:204:TYR:HB2	2.30	0.66
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.77	0.66
1:A:583:ASN:HD21	1:A:585:ARG:HD2	1.61	0.66
1:B:312:ARG:O	1:B:316:GLU:HG3	1.97	0.65
1:A:195:ILE:O	1:A:196:PHE:HD2	1.79	0.65
1:B:228:GLU:O	1:B:231:ARG:HG2	1.97	0.65
1:B:467:ASP:CG	1:B:470:ARG:HH12	2.00	0.65
1:A:409:ALA:O	1:A:413:LEU:HD13	1.96	0.64
1:A:374:TYR:CE1	1:A:375:LEU:HD13	2.33	0.64
1:A:92:GLU:O	1:A:92:GLU:HG2	1.97	0.64
1:A:326:VAL:HG12	1:A:329:GLU:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ASP:OD1	1:B:579:MET:HG2	1.98	0.64
1:B:228:GLU:OE2	1:B:231:ARG:HD3	1.96	0.64
1:B:504:ASN:HD22	1:B:504:ASN:C	2.00	0.63
1:A:515:ASN:ND2	1:A:534:ASN:HB3	2.12	0.63
1:A:31:LYS:HE2	1:A:63:ASP:O	2.00	0.62
1:A:195:ILE:HG13	1:A:195:ILE:O	2.00	0.61
1:A:426:LEU:HD23	1:A:461:ALA:HB2	1.81	0.61
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.47	0.61
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.31	0.61
1:B:453:TYR:HB3	1:B:456:ASP:OD2	2.01	0.61
1:B:353:GLY:O	1:B:371:VAL:HA	2.01	0.61
1:A:253:ARG:HA	1:A:256:LEU:HD12	1.83	0.60
1:A:381:ILE:O	1:A:385:ALA:HB3	2.02	0.60
1:B:143:ASN:ND2	1:B:169:GLY:HA3	2.16	0.60
1:A:183:GLU:OE2	1:A:232:ARG:HD3	2.02	0.60
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.84	0.60
1:A:551:LYS:HG3	1:A:552:THR:HG23	1.84	0.59
1:A:84:PHE:O	1:A:95:TYR:HA	2.01	0.59
1:A:140:ARG:HG2	1:A:469:ARG:O	2.02	0.59
1:A:162:PRO:CG	1:A:470:ARG:HA	2.33	0.58
1:A:535:ARG:HH21	1:A:535:ARG:HG3	1.68	0.58
1:A:441:LEU:HD22	1:A:532:LEU:HD21	1.84	0.58
1:A:582:TRP:CE2	1:A:584:GLY:HA2	2.38	0.58
1:B:455:GLY:O	1:B:458:ILE:HG13	2.04	0.58
1:A:258:LYS:HB3	1:A:261:GLN:HB2	1.85	0.58
1:B:458:ILE:HD11	1:B:460:MET:HG3	1.85	0.58
1:A:218:ASP:OD1	1:A:220:PRO:HD2	2.03	0.58
1:A:255:VAL:HA	1:A:262:SER:HG	1.70	0.57
1:B:82:TYR:O	1:B:110:VAL:HG23	2.03	0.57
1:B:390:HIS:CE1	1:B:392:GLU:HB2	2.38	0.57
1:A:514:ALA:HB1	1:A:539:GLN:NE2	2.19	0.57
1:B:127:TRP:CD2	1:B:235:LYS:HE3	2.39	0.57
1:B:36:ARG:HB3	1:B:87:THR:HB	1.85	0.57
1:A:134:TYR:HB2	1:A:187:VAL:HG11	1.86	0.57
1:B:447:LEU:HB2	1:B:505:VAL:HG21	1.85	0.56
1:B:136:ILE:HD12	1:B:190:LEU:HG	1.86	0.56
1:B:31:LYS:HG2	1:B:67:ASP:OD1	2.05	0.56
1:A:416:LEU:H	1:A:416:LEU:CD2	2.18	0.56
1:A:277:LYS:HB2	1:A:277:LYS:NZ	2.20	0.56
1:A:574:ARG:HH11	1:A:574:ARG:HB3	1.70	0.56
1:B:240:ALA:HB1	1:B:242:PHE:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLY:HA2	1:B:275:VAL:CG2	2.35	0.56
1:B:436:PHE:HE2	1:B:483:LEU:HD21	1.70	0.56
1:B:465:ASP:OD2	1:B:466:PRO:HA	2.05	0.56
1:A:105:ARG:HG3	1:A:106:SER:N	2.21	0.56
1:B:84:PHE:HB2	1:B:96:PHE:HB3	1.87	0.56
1:A:11:LYS:N	1:A:15:ALA:HB3	2.21	0.55
1:B:43:ASP:O	1:B:81:LYS:HE2	2.06	0.55
1:A:122:PHE:O	1:A:408:GLN:HG2	2.07	0.55
1:A:141:PHE:HD1	1:A:175:VAL:HG22	1.73	0.54
1:B:522:THR:HG23	1:B:527:HIS:CD2	2.43	0.54
1:A:544:GLN:CD	1:A:544:GLN:N	2.61	0.54
1:B:300:ASN:OD1	1:B:302:GLU:N	2.41	0.54
1:B:183:GLU:OE2	1:B:232:ARG:HG3	2.07	0.54
1:B:139:GLU:OE2	1:B:140:ARG:NH1	2.40	0.54
1:B:518:ALA:HA	1:B:530:VAL:O	2.07	0.54
1:B:82:TYR:C	1:B:110:VAL:HG23	2.29	0.54
1:A:544:GLN:N	1:A:544:GLN:OE1	2.40	0.54
1:A:278:THR:O	1:A:279:SER:HB3	2.07	0.54
1:A:82:TYR:N	1:A:110:VAL:HG23	2.23	0.54
1:A:570:LYS:O	1:A:571:LEU:HD12	2.07	0.54
1:A:346:ASN:HB3	1:A:349:ALA:HB2	1.89	0.53
1:A:162:PRO:CD	1:A:470:ARG:HG2	2.38	0.53
1:A:276:SER:O	1:A:277:LYS:HB2	2.08	0.53
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.89	0.53
1:A:583:ASN:ND2	1:A:585:ARG:HD2	2.23	0.53
1:B:26:ARG:NE	1:B:70:GLU:OE2	2.41	0.52
1:B:138:PRO:HG3	1:B:195:ILE:CG2	2.39	0.52
1:A:133:ILE:N	1:A:133:ILE:HD12	2.23	0.52
1:A:202:HIS:HB2	1:A:204:TYR:HD2	1.74	0.52
1:B:332:HIS:HD2	1:B:367:GLN:HE22	1.56	0.52
1:A:523:VAL:HG13	1:A:523:VAL:O	2.09	0.52
1:B:332:HIS:CD2	1:B:367:GLN:HE22	2.28	0.52
1:A:135:GLN:HG3	1:A:191:TYR:CD2	2.45	0.52
1:B:197:ALA:HB3	1:B:208:ASP:HB3	1.92	0.51
1:B:497:LEU:HB2	1:B:500:LEU:HD12	1.91	0.51
1:A:309:ASP:OD2	1:A:312:ARG:NH1	2.43	0.51
1:B:240:ALA:HB2	1:B:322:TRP:CE3	2.45	0.51
1:B:153:THR:HA	1:B:167:PHE:O	2.10	0.51
1:A:390:HIS:HD2	1:A:392:GLU:H	1.57	0.51
1:B:389:ILE:HB	1:B:393:ARG:HG2	1.93	0.51
1:A:1:MET:HB2	1:A:33:ASP:OD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:PHE:CG	1:B:251:ALA:N	2.79	0.51
1:A:202:HIS:HB2	1:A:204:TYR:CD2	2.46	0.51
1:A:139:GLU:OE2	1:A:140:ARG:NH1	2.42	0.50
1:A:275:VAL:O	1:A:276:SER:CB	2.57	0.50
1:B:273:PHE:HA	1:B:274:PRO:C	2.32	0.50
1:B:244:HIS:CD2	1:B:286:TYR:HB2	2.47	0.50
1:A:206:THR:HG21	1:A:209:TYR:CD2	2.46	0.50
1:B:193:THR:O	1:B:195:ILE:HG23	2.11	0.50
1:B:352:VAL:HG21	1:B:414:TRP:CZ2	2.46	0.50
1:B:8:HIS:CG	1:B:9:GLU:N	2.79	0.50
1:A:488:LYS:HB3	1:A:492:ARG:HH12	1.77	0.50
1:B:545:VAL:HG21	1:B:569:LEU:HD13	1.93	0.50
1:B:137:PHE:HE1	1:B:469:ARG:HH11	1.58	0.50
1:A:544:GLN:CD	1:A:544:GLN:H	2.14	0.50
1:A:133:ILE:HD13	1:A:449:THR:HG21	1.94	0.50
1:B:438:LEU:HD11	1:B:532:LEU:HB3	1.93	0.50
1:B:144:GLY:HA3	1:B:173:LYS:HG3	1.94	0.49
1:A:232:ARG:HH21	1:A:232:ARG:HG3	1.77	0.49
1:B:2:LEU:N	1:B:33:ASP:OD2	2.44	0.49
1:B:315:MET:HA	1:B:319:ILE:HG12	1.95	0.49
1:A:335:TRP:CE3	1:A:335:TRP:HA	2.48	0.49
1:A:304:LYS:HG2	1:A:308:PHE:CE1	2.48	0.49
1:A:92:GLU:CG	1:A:92:GLU:O	2.60	0.49
1:A:44:ARG:HA	1:A:81:LYS:HD3	1.94	0.49
1:B:271:GLU:N	1:B:271:GLU:OE2	2.46	0.49
1:B:436:PHE:CE2	1:B:483:LEU:HD21	2.48	0.49
1:A:200:SER:OG	1:A:202:HIS:CE1	2.66	0.49
1:B:255:VAL:HA	1:B:262:SER:HB2	1.95	0.49
1:B:467:ASP:CG	1:B:470:ARG:NH1	2.66	0.49
1:B:504:ASN:ND2	1:B:504:ASN:C	2.66	0.49
1:B:218:ASP:OD2	1:B:220:PRO:HD2	2.12	0.49
1:A:118:ARG:NH2	1:B:297:ARG:HH12	2.11	0.49
1:B:494:ARG:HG3	1:B:494:ARG:NH1	2.28	0.49
1:B:547:GLU:OE1	1:B:551:LYS:HD2	2.12	0.49
1:B:323:ARG:HD2	1:B:323:ARG:C	2.33	0.49
1:B:137:PHE:HE1	1:B:469:ARG:NH1	2.11	0.49
1:A:82:TYR:O	1:A:110:VAL:HG23	2.12	0.49
1:A:356:TRP:HA	1:A:356:TRP:CE3	2.48	0.49
1:A:195:ILE:CG1	1:A:195:ILE:O	2.59	0.48
1:A:82:TYR:N	1:A:110:VAL:CG2	2.75	0.48
1:A:162:PRO:HD3	1:A:470:ARG:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:ALA:O	1:B:535:ARG:HD2	2.14	0.48
1:A:228:GLU:OE2	1:A:231:ARG:HD3	2.13	0.48
1:A:384:PHE:O	1:A:435:LYS:HD3	2.12	0.48
1:A:516:LEU:HD22	1:A:541:VAL:HG11	1.96	0.48
1:A:197:ALA:CB	1:A:208:ASP:HB3	2.38	0.48
1:B:357:HIS:HA	1:B:374:TYR:OH	2.13	0.48
1:B:193:THR:HB	1:B:194:PRO:HD2	1.96	0.48
1:A:432:ASN:OD1	1:A:434:ALA:N	2.46	0.48
1:A:356:TRP:HE3	1:A:356:TRP:HA	1.77	0.48
1:B:271:GLU:OE2	1:B:283:TYR:HA	2.14	0.48
1:B:40:LEU:HD22	1:B:54:HIS:CE1	2.49	0.48
1:A:7:PHE:CZ	1:A:9:GLU:HG2	2.49	0.48
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.96	0.48
1:A:504:ASN:HD21	1:A:522:THR:HB	1.79	0.48
1:B:193:THR:O	1:B:194:PRO:C	2.52	0.48
1:A:574:ARG:HB3	1:A:574:ARG:NH1	2.29	0.48
1:B:118:ARG:HA	1:B:121:VAL:HG23	1.96	0.48
1:A:357:HIS:HB2	1:B:98:GLU:OE2	2.13	0.48
1:A:416:LEU:HB3	1:A:451:LEU:HD23	1.96	0.47
1:B:281:THR:HG21	1:B:289:GLN:HA	1.96	0.47
1:B:416:LEU:H	1:B:416:LEU:HD23	1.79	0.47
1:B:140:ARG:HD2	1:B:469:ARG:O	2.13	0.47
1:B:16:TYR:CE2	1:B:406:PRO:HA	2.49	0.47
1:A:23:LEU:HD22	1:A:80:VAL:HG11	1.96	0.47
1:A:271:GLU:HG3	1:A:272:ASP:OD2	2.13	0.47
1:B:312:ARG:HG3	1:B:312:ARG:NH2	2.29	0.47
1:A:492:ARG:HD2	1:A:496:ARG:NH1	2.29	0.47
1:A:525:ASP:O	1:A:585:ARG:HD2	2.14	0.47
1:B:494:ARG:HH11	1:B:494:ARG:HG3	1.78	0.47
1:A:249:PHE:CE2	1:A:251:ALA:HB3	2.50	0.47
1:A:270:ILE:HD13	1:A:275:VAL:HG21	1.96	0.47
1:B:77:THR:O	1:B:79:ARG:HG3	2.14	0.47
1:B:312:ARG:HG3	1:B:312:ARG:HH21	1.80	0.47
1:B:385:ALA:HB1	1:B:428:SER:O	2.15	0.47
1:B:22:GLN:HB3	1:B:72:LEU:HD11	1.97	0.47
1:A:300:ASN:OD1	1:A:301:PRO:HD2	2.15	0.47
1:B:243:ASN:HD22	1:B:329:GLU:HB2	1.80	0.47
1:A:82:TYR:C	1:A:110:VAL:HG23	2.36	0.46
1:A:7:PHE:CG	1:A:8:HIS:N	2.83	0.46
1:B:259:GLY:HA2	1:B:275:VAL:HG21	1.98	0.46
1:A:504:ASN:N	1:A:504:ASN:HD22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:LEU:N	1:A:573:LEU:HD22	2.30	0.46
1:A:457:GLU:HG2	1:A:458:ILE:N	2.29	0.46
1:A:488:LYS:HB3	1:A:492:ARG:NH1	2.30	0.46
1:B:137:PHE:HD2	1:B:138:PRO:HD2	1.81	0.46
1:B:7:PHE:CD2	1:B:28:ARG:CZ	2.99	0.46
1:A:478:GLU:HA	1:A:478:GLU:OE2	2.16	0.46
1:B:146:PRO:HA	1:B:149:ASP:OD2	2.15	0.46
1:B:381:ILE:HG12	1:B:425:PHE:HE1	1.81	0.46
1:B:285:THR:HB	1:B:293:MET:O	2.16	0.46
1:B:269:PHE:CE2	1:B:295:LYS:HG2	2.50	0.46
1:B:487:TYR:O	1:B:491:ILE:HG13	2.16	0.46
1:B:253:ARG:HH11	1:B:253:ARG:HB3	1.81	0.46
1:A:535:ARG:HG3	1:A:535:ARG:NH2	2.30	0.46
1:B:206:THR:HG21	1:B:209:TYR:CD2	2.51	0.46
1:A:24:ARG:HD2	1:A:70:GLU:CG	2.45	0.46
1:A:373:ASN:O	1:A:376:PHE:HB3	2.16	0.45
1:A:382:ARG:HA	1:A:386:THR:OG1	2.16	0.45
1:B:193:THR:HB	1:B:194:PRO:CD	2.47	0.45
1:A:373:ASN:HB2	1:A:413:LEU:HB3	1.98	0.45
1:A:464:THR:OG1	1:A:465:ASP:N	2.49	0.45
1:A:486:PHE:CZ	1:A:490:LEU:HD11	2.51	0.45
1:A:499:SER:HB3	1:A:523:VAL:HG12	1.98	0.45
1:B:330:VAL:HB	1:B:335:TRP:NE1	2.31	0.45
1:A:326:VAL:O	1:A:326:VAL:HG12	2.15	0.45
1:A:10:ALA:O	1:A:11:LYS:HB3	2.16	0.45
1:A:230:HIS:C	1:A:232:ARG:N	2.69	0.45
1:A:122:PHE:HE1	1:A:363:LEU:O	1.99	0.45
1:A:327:ALA:O	1:A:330:VAL:HG13	2.17	0.45
1:B:241:VAL:HG13	1:B:325:ASP:HB3	1.99	0.45
1:B:228:GLU:O	1:B:232:ARG:HD3	2.17	0.45
1:B:381:ILE:HG12	1:B:425:PHE:CE1	2.51	0.45
1:B:582:TRP:CE2	1:B:584:GLY:HA2	2.52	0.45
1:B:377:ARG:CZ	1:B:381:ILE:HD11	2.46	0.45
1:B:140:ARG:HG3	1:B:469:ARG:HB3	1.99	0.45
1:B:493:LEU:HD21	1:B:556:CYS:HB3	1.99	0.45
1:A:357:HIS:O	1:A:358:ASP:C	2.55	0.45
1:A:427:THR:O	1:A:430:GLY:N	2.45	0.45
1:B:18:ILE:HD12	1:B:19:SER:HB3	1.98	0.45
1:B:533:ASN:O	1:B:576:TYR:HA	2.16	0.45
1:B:504:ASN:O	1:B:521:ARG:HA	2.17	0.44
1:B:245:ALA:O	1:B:294:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:N	1:B:180:PRO:CD	2.80	0.44
1:A:573:LEU:CD1	1:A:579:MET:SD	3.05	0.44
1:B:202:HIS:O	1:B:203:LYS:HB2	2.17	0.44
1:B:464:THR:O	1:B:465:ASP:C	2.55	0.44
1:A:7:PHE:CD2	1:A:28:ARG:NH1	2.86	0.44
1:B:92:GLU:H	1:B:92:GLU:CD	2.21	0.44
1:B:218:ASP:HB2	1:B:220:PRO:HD2	1.99	0.44
1:A:209:TYR:HB3	1:A:310:VAL:HG11	1.98	0.44
1:B:533:ASN:HB2	1:B:573:LEU:CB	2.47	0.44
1:A:176:ILE:HA	1:A:179:LEU:HG	1.99	0.44
1:A:306:TYR:O	1:A:310:VAL:HG23	2.17	0.44
1:A:112:GLN:HB2	1:B:357:HIS:CD2	2.53	0.44
1:B:437:ARG:HB3	1:B:486:PHE:CE1	2.53	0.44
1:B:315:MET:HG2	1:B:319:ILE:HD11	1.99	0.44
1:B:246:GLY:HA2	1:B:292:ALA:O	2.18	0.44
1:A:381:ILE:HD13	1:A:425:PHE:CE1	2.53	0.44
1:A:8:HIS:CG	1:A:9:GLU:N	2.86	0.44
1:B:245:ALA:O	1:B:293:MET:HA	2.18	0.43
1:A:282:ASN:C	1:A:282:ASN:HD22	2.22	0.43
1:B:190:LEU:HD13	1:B:234:ILE:CG2	2.48	0.43
1:B:553:TRP:HB3	1:B:581:LEU:HB3	2.00	0.43
1:B:455:GLY:HA2	1:B:472:MET:SD	2.59	0.43
1:B:110:VAL:HG22	1:B:111:PHE:O	2.18	0.43
1:A:198:SER:HB3	1:A:203:LYS:HD2	2.00	0.43
1:A:127:TRP:O	1:A:131:ALA:HB2	2.18	0.43
1:A:6:ILE:HD13	1:A:86:LEU:HD13	2.01	0.43
1:A:277:LYS:HG2	1:A:280:ARG:HB3	1.99	0.43
1:A:133:ILE:HD13	1:A:449:THR:CG2	2.48	0.43
1:A:465:ASP:OD1	1:A:466:PRO:HA	2.19	0.43
1:A:127:TRP:CG	1:A:235:LYS:HE2	2.54	0.43
1:A:191:TYR:CE1	1:A:323:ARG:HG3	2.54	0.43
1:B:121:VAL:O	1:B:122:PHE:C	2.56	0.43
1:B:285:THR:HG22	1:B:294:PRO:HA	2.00	0.43
1:A:453:TYR:HB3	1:A:456:ASP:OD2	2.18	0.43
1:A:343:LYS:HE2	1:A:349:ALA:O	2.19	0.43
1:A:504:ASN:ND2	1:A:522:THR:HB	2.33	0.43
1:A:352:VAL:HG21	1:A:414:TRP:CZ2	2.53	0.43
1:A:307:LEU:HD12	1:A:334:PHE:CE2	2.53	0.43
1:B:26:ARG:HA	1:B:69:PHE:O	2.19	0.43
1:B:271:GLU:HB2	1:B:282:ASN:O	2.19	0.43
1:A:457:GLU:HA	1:A:487:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLY:HA2	1:A:364:MET:SD	2.59	0.43
1:A:545:VAL:HG21	1:A:569:LEU:HB2	2.00	0.43
1:A:191:TYR:HA	1:A:237:ILE:HB	2.01	0.42
1:B:426:LEU:HD23	1:B:461:ALA:HB2	2.01	0.42
1:A:264:TYR:HD2	1:A:267:TRP:CE2	2.37	0.42
1:B:465:ASP:HA	1:B:466:PRO:HA	1.89	0.42
1:B:37:CYS:O	1:B:57:ALA:HB3	2.19	0.42
1:A:475:GLU:OE1	1:A:477:LYS:HB2	2.18	0.42
1:A:96:PHE:CD2	1:A:101:PHE:CZ	3.08	0.42
1:B:276:SER:HA	1:B:282:ASN:OD1	2.18	0.42
1:A:78:LYS:HE3	1:A:115:TYR:OH	2.20	0.42
1:A:232:ARG:NH2	1:A:232:ARG:HG3	2.34	0.42
1:B:190:LEU:HD13	1:B:234:ILE:HG21	2.01	0.42
1:B:278:THR:C	1:B:280:ARG:H	2.23	0.42
1:A:75:CYS:SG	1:A:80:VAL:HB	2.58	0.42
1:B:330:VAL:HG11	1:B:334:PHE:CD1	2.55	0.42
1:A:14:TYR:HA	1:A:26:ARG:HB2	2.00	0.42
1:A:574:ARG:NH1	1:A:574:ARG:CB	2.83	0.42
1:B:206:THR:HG21	1:B:209:TYR:CG	2.55	0.42
1:A:255:VAL:HG22	1:A:262:SER:CB	2.49	0.42
1:B:424:ARG:NH1	1:B:454:TYR:O	2.42	0.42
1:A:446:TYR:CG	1:A:447:LEU:N	2.88	0.42
1:B:499:SER:OG	1:B:526:GLN:OE1	2.21	0.42
1:B:398:LEU:HD21	1:B:442:PHE:CZ	2.55	0.42
1:B:373:ASN:ND2	1:B:376:PHE:HB2	2.34	0.42
1:B:40:LEU:CD2	1:B:54:HIS:ND1	2.83	0.41
1:B:178:ARG:HD2	1:B:474:TRP:CZ3	2.55	0.41
1:A:193:THR:HB	1:A:194:PRO:CD	2.49	0.41
1:B:358:ASP:OD1	1:B:358:ASP:C	2.58	0.41
1:A:245:ALA:O	1:A:294:PRO:HD2	2.20	0.41
1:B:355:ILE:CG2	1:B:357:HIS:CE1	3.03	0.41
1:A:134:TYR:CE2	1:A:136:ILE:CD1	3.03	0.41
1:A:110:VAL:HG22	1:A:111:PHE:O	2.20	0.41
1:B:9:GLU:OE2	1:B:11:LYS:HE3	2.19	0.41
1:B:280:ARG:HD2	1:B:281:THR:N	2.36	0.41
1:B:377:ARG:O	1:B:380:VAL:HG22	2.19	0.41
1:A:480:ASN:OD1	1:A:483:LEU:HB2	2.20	0.41
1:B:309:ASP:HA	1:B:312:ARG:HH21	1.83	0.41
1:A:137:PHE:HD1	1:A:140:ARG:HB2	1.86	0.41
1:A:484:PHE:O	1:A:488:LYS:HG3	2.20	0.41
1:A:281:THR:OG1	1:A:289:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:GLU:OE2	1:B:562:VAL:HG12	2.20	0.41
1:A:52:LEU:HD12	1:A:105:ARG:HH11	1.86	0.41
1:A:312:ARG:NE	1:A:341:LEU:HD11	2.34	0.41
1:B:384:PHE:CE2	1:B:438:LEU:HD12	2.55	0.41
1:A:579:MET:HE2	1:A:579:MET:HB3	1.87	0.41
1:A:141:PHE:CD1	1:A:175:VAL:HG22	2.54	0.41
1:A:454:TYR:CD1	1:A:454:TYR:C	2.93	0.41
1:A:36:ARG:HH11	1:A:36:ARG:HG2	1.85	0.41
1:B:158:LYS:HD2	1:B:478:GLU:HB3	2.02	0.41
1:A:270:ILE:HG21	1:A:275:VAL:HG22	2.03	0.41
1:A:202:HIS:O	1:A:203:LYS:HB2	2.21	0.41
1:B:535:ARG:HD3	1:B:539:GLN:OE1	2.20	0.41
1:B:16:TYR:O	1:B:16:TYR:CD1	2.73	0.41
1:B:356:TRP:CZ3	1:B:374:TYR:HB3	2.56	0.41
1:B:219:LEU:HD11	1:B:317:GLN:OE1	2.21	0.41
1:A:271:GLU:HG3	1:A:272:ASP:CG	2.41	0.41
1:B:172:LEU:HG	1:B:216:PHE:HB3	2.03	0.41
1:B:335:TRP:HA	1:B:335:TRP:CE3	2.56	0.41
1:B:464:THR:OG1	1:B:465:ASP:N	2.54	0.41
1:A:264:TYR:O	1:A:267:TRP:HB2	2.20	0.41
1:B:449:THR:HA	1:B:450:PRO:HD3	1.92	0.41
1:A:377:ARG:HD2	1:A:417:LEU:C	2.41	0.41
1:A:389:ILE:HB	1:A:393:ARG:HG2	2.02	0.41
1:A:314:TRP:O	1:A:319:ILE:HG12	2.20	0.41
1:B:526:GLN:C	1:B:527:HIS:HD2	2.23	0.41
1:B:569:LEU:CD2	1:B:571:LEU:HD21	2.46	0.41
1:A:374:TYR:CE1	1:A:375:LEU:CD1	3.03	0.41
1:B:82:TYR:N	1:B:110:VAL:CG2	2.84	0.41
1:B:332:HIS:HD2	1:B:367:GLN:NE2	2.18	0.41
1:A:249:PHE:CD2	1:A:251:ALA:HB3	2.55	0.41
1:B:7:PHE:CD2	1:B:28:ARG:NH1	2.89	0.41
1:A:27:LEU:C	1:A:27:LEU:HD23	2.42	0.41
1:B:232:ARG:CG	1:B:232:ARG:HH11	2.34	0.40
1:B:389:ILE:HB	1:B:393:ARG:CG	2.50	0.40
1:B:243:ASN:ND2	1:B:329:GLU:HB2	2.35	0.40
1:A:273:PHE:HA	1:A:274:PRO:C	2.42	0.40
1:B:17:PRO:HA	1:B:23:LEU:HA	2.03	0.40
1:B:6:ILE:HA	1:B:28:ARG:O	2.21	0.40
1:B:158:LYS:HD3	1:B:478:GLU:OE1	2.21	0.40
1:B:242:PHE:N	1:B:242:PHE:CD1	2.88	0.40
1:A:465:ASP:HA	1:A:466:PRO:HA	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:TYR:CD1	1:A:375:LEU:HD13	2.56	0.40
1:B:339:ARG:HD2	1:B:367:GLN:O	2.21	0.40
1:B:454:TYR:CG	1:B:454:TYR:O	2.74	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	583/585 (100%)	551 (94%)	28 (5%)	4 (1%)	26	72
1	B	583/585 (100%)	552 (95%)	30 (5%)	1 (0%)	52	88
All	All	1166/1170 (100%)	1103 (95%)	58 (5%)	5 (0%)	39	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	SER
1	A	547	GLU
1	B	547	GLU
1	A	277	LYS
1	A	195	ILE

5.3.2 Protein sidechains [i](#)

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	493/493 (100%)	455 (92%)	38 (8%)	16	54
1	B	493/493 (100%)	462 (94%)	31 (6%)	22	63
All	All	986/986 (100%)	917 (93%)	69 (7%)	19	58

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	38	GLU
1	A	40	LEU
1	A	62	SER
1	A	65	ARG
1	A	77	THR
1	A	92	GLU
1	A	105	ARG
1	A	122	PHE
1	A	130	GLU
1	A	139	GLU
1	A	155	GLN
1	A	159	ASP
1	A	164	HIS
1	A	167	PHE
1	A	188	THR
1	A	193	THR
1	A	219	LEU
1	A	221	THR
1	A	223	ARG
1	A	263	ARG
1	A	272	ASP
1	A	277	LYS
1	A	282	ASN
1	A	323	ARG
1	A	325	ASP
1	A	330	VAL
1	A	346	ASN
1	A	375	LEU
1	A	411	GLN
1	A	422	THR
1	A	444	MET
1	A	454	TYR
1	A	483	LEU
1	A	504	ASN

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Mol	Chain	Res	Type
1	A	544	GLN
1	A	545	VAL
1	A	547	GLU
1	B	13	SER
1	B	52	LEU
1	B	64	GLU
1	B	122	PHE
1	B	139	GLU
1	B	167	PHE
1	B	202	HIS
1	B	232	ARG
1	B	241	VAL
1	B	248	GLN
1	B	250	PHE
1	B	255	VAL
1	B	261	GLN
1	B	265	LYS
1	B	277	LYS
1	B	323	ARG
1	B	325	ASP
1	B	328	ASN
1	B	337	GLU
1	B	340	ARG
1	B	364	MET
1	B	398	LEU
1	B	411	GLN
1	B	438	LEU
1	B	451	LEU
1	B	464	THR
1	B	467	ASP
1	B	475	GLU
1	B	504	ASN
1	B	552	THR
1	B	569	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	135	GLN
1	A	155	GLN
1	A	244	HIS

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Mol	Chain	Res	Type
1	A	282	ASN
1	A	289	GLN
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN
1	A	390	HIS
1	A	411	GLN
1	A	504	ASN
1	A	526	GLN
1	A	527	HIS
1	A	539	GLN
1	B	135	GLN
1	B	257	GLN
1	B	261	GLN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	367	GLN
1	B	411	GLN
1	B	495	HIS
1	B	504	ASN
1	B	524	GLN
1	B	527	HIS
1	B	534	ASN
1	B	539	GLN
1	B	544	GLN
1	B	566	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 2 ligands modelled in this entry, 2 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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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