



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:54 AM GMT

PDB ID : 1DDN  
Title : DIPHTHERIA TOX REPRESSOR (C102D MUTANT)/TOX DNA OPERATOR COMPLEX  
Authors : White, A.; Ding, X.; Vanderspek, J.C.; Murphy, J.R.; Ringe, D.  
Deposited on : 1998-06-23  
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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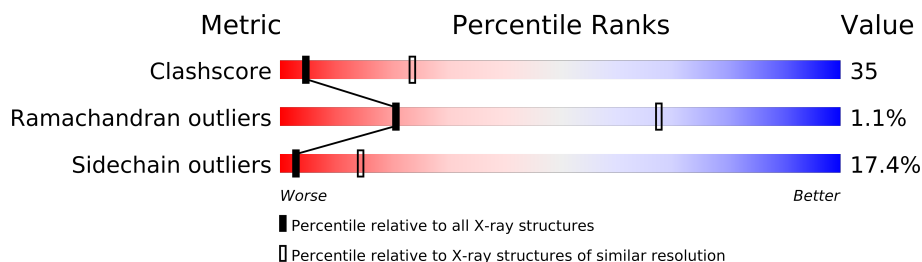
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

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  $\geq 3$ , 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	E	33	
2	F	33	
3	A	226	
3	B	226	
3	C	226	
3	D	226	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5135 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 DNA chain called 33 BASE DNA CONTAINING TOXIN OPERATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	33	Total	C	N	O	P	0	0	0
			672	327	114	199	32			

- Molecule 2 is a DNA chain called 33 BASE DNA CONTAINING TOXIN OPERATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	33	Total	C	N	O	P	0	0	0
			675	327	123	193	32			

- Molecule 3 is a protein called DIPHTHERIA TOX REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	118	Total	C	N	O	S	0	0	0
			944	581	174	184	5			
3	B	118	Total	C	N	O	S	0	0	0
			944	581	174	184	5			
3	C	118	Total	C	N	O	S	0	0	0
			944	581	174	184	5			
3	D	118	Total	C	N	O	S	0	0	0
			944	581	174	184	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ASP	CYS	ENGINEERED	UNP P33120
B	102	ASP	CYS	ENGINEERED	UNP P33120
C	102	ASP	CYS	ENGINEERED	UNP P33120
D	102	ASP	CYS	ENGINEERED	UNP P33120

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ni 2 2	0	0
4	A	2	Total Ni 2 2	0	0
4	D	2	Total Ni 2 2	0	0
4	C	2	Total Ni 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0



GLY	VAL	GLY	ASN	SER	ASP	ALA	ALA	ALA	GLY	THR	ARG	VAL	ILE	ASP	ALA	ALA	SER	THR	SER	MET	PRO	ARG	LYS	VAL	ARG	ILE	ILE	PHE	PHE	GLN	GLN	VAL	GLU	THR	ASP	ASP	GLN	PHE	THR	GLN	LEU	LEU	ASP	ALA	ASP	ILE	ARG	VAL	VAL	GLY	SER	GLU	VAL	GLU	ILE	VAL	VAL	ASP	ASP
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ASP GLY HIS HIS ILE THR LEU SER HIS ASN GLY LYS ASP VAL GLU LEU LEU ASP ASP LEU LEU ALA HIS THR THR ILE ARG ILE GLU GLU LEU LEU

- Molecule 3: DIPHTHERIA TOX REPRESSOR

Chain C:

MET	LVS	D3	L4	V5	D6	T7	T8		R13		Y16	E17	L18	E21	G22	V23	T24		R27	A28	R29	I30	A31	E32	R33	L34		S37	G38	P39	T40	V41	S42	Q43	L44	V45	A46		V54	V55		S58	D59	R60		R69	T70	L71	A72		M76		H79		A82	E83	R84		R85
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L66	L67	L68	L69	L70	L71	L72	L73	L74	L75	L76	L77	L78	L79	L80	L81	L82	L83	L84	L85	L86	L87	L88	L89	L90	L91	L92	L93	L94	L95	L96	L97	L98	L99	L100	L101	L102	L103	L104	L105	L106	L107	L108	L109	L110	L111	L112	L113	L114	L115	L116	L117	L118	L119	L120	L121	L122	L123	L124	L125	L126	L127	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180	L181	L182	L183	L184	L185	L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580
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THR	ARG	VAL	ASP	ALA	ALA	THR	SER	MET	PRO	LYS	ARG	VAL	GLN	ILE	GLU	ILE	PHE	GLN	VAL	GLU	THR	ASP	GLN	PHE	THR	GLN	LEU	ASP	ALA	ASP	ILE	ARG	VAL	VAL	GLY	SER	GLU	VAL	GLU	ILE	ILE	VAL	ASP	VAL	ARG	ASP	GLY	HIS	ILE	THR	LEU	SER	HIS	ASN	GLY	LYS
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ASP  
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GLU  
GLU  
LEU

- Molecule 3: DIPHTHERIA TOX REPRESSOR

Chain D:

Met	D3	D5	D6	M10	L12	L15	L16	E17	E20	E21	L26	R27	A28	R29	E32	R33	L34	S37	G38	P39	L40	V41	S42	Q43	T44	V45	A46	R47	M48	E49	R50	D51	L53	G52	V54	A57	S58	D59	R60	S61	L62	Q63	M64	T67	G68	R69	T70	L71
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A72	T73	H79	A82	E83	R84	L85	L86	T87	D88	I89	R90	L92	D93	I94	R95	E96	V97	H98	R99	E100	A101	V104	E105	H106	V107	E111	R114	R115	L116	V117	K118	V119	L120	LVS	ASP	VAL	SER	SER	ARG	ARG	PRO	PRO	PHE	GLY	GLY	PRO	PRO	ASP	ASP	GLU	GLU	LEU	LEU	GLY	VAL
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GLY	ASN	SER	ASP	ALA	ALA	PRO	GLY	THR	ARG	VAL	ILE	ASP	ALA	ALA	THR	SER	MET	PRO	ARG	LYS	VAL	ARG	ILE	VAL	GLN	ASN	GLU	ILE	PHE	GLN	VAL	GLU	THR	THR	GLN	LEU	LEU	ASP	ALA	ASP	ILE	ARG	VAL	GLY	SER	GLU	VAL	GLU	ILE	GLU	ILE	ASP	LYS
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HIS	ILE	THR	LEU	SER	HIS	ASN	GLY	LYS	ASP	VAL	GLU	LEU	LEU	ASP	ASP	LEU	ALA	HIS	THR	ILE	ARG	ILE	GLU	GLU	LEU
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.05Å 117.05Å 145.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	87.9 (8.00-3.00)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.240 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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: NI

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	E	0.81	3/752 (0.4%)	1.26	14/1159 (1.2%)
2	F	0.69	0/758	1.23	11/1168 (0.9%)
3	A	0.42	0/953	0.65	0/1288
3	B	0.39	0/953	0.61	0/1288
3	C	0.39	0/953	0.64	0/1288
3	D	0.39	0/953	0.63	0/1288
All	All	0.52	3/5322 (0.1%)	0.87	25/7479 (0.3%)

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	E	0	5
2	F	0	6
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	317	DT	C5-C6	-6.29	1.29	1.34
1	E	317	DT	C5-C7	5.97	1.53	1.50
1	E	317	DT	N1-C6	-5.44	1.34	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	413	DG	O4'-C1'-N9	8.18	113.73	108.00
1	E	310	DG	O4'-C1'-N9	7.95	113.56	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	424	DC	C6-N1-C2	7.81	123.42	120.30
1	E	311	DG	N9-C1'-C2'	-7.70	97.97	112.60
2	F	419	DG	O4'-C1'-N9	7.43	113.20	108.00
2	F	424	DC	O4'-C1'-N1	7.33	113.13	108.00
1	E	316	DC	O4'-C1'-N1	7.20	113.04	108.00
1	E	317	DT	C6-N1-C2	7.20	124.90	121.30
2	F	420	DC	O4'-C1'-N1	7.03	112.92	108.00
1	E	317	DT	C6-C5-C7	-6.70	118.88	122.90
2	F	425	DC	O4'-C1'-N1	6.26	112.38	108.00
1	E	317	DT	N1-C1'-C2'	-6.19	100.84	112.60
1	E	322	DC	C6-N1-C2	5.56	122.52	120.30
1	E	322	DC	O4'-C1'-N1	5.53	111.87	108.00
2	F	402	DT	C6-C5-C7	-5.49	119.61	122.90
1	E	321	DC	O4'-C1'-N1	5.46	111.82	108.00
2	F	401	DT	C6-C5-C7	-5.42	119.65	122.90
1	E	316	DC	C6-N1-C2	5.40	122.46	120.30
1	E	331	DT	C4-C5-C6	5.38	121.23	118.00
2	F	419	DG	N9-C1'-C2'	-5.34	102.46	112.60
2	F	401	DT	C4-C5-C6	5.22	121.14	118.00
1	E	332	DT	C4-C5-C6	5.21	121.13	118.00
1	E	321	DC	C6-N1-C2	5.20	122.38	120.30
2	F	402	DT	C4-C5-C6	5.18	121.11	118.00
1	E	332	DT	C5-C6-N1	-5.03	120.68	123.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	310	DG	Sidechain
1	E	311	DG	Sidechain
1	E	316	DC	Sidechain
1	E	321	DC	Sidechain
1	E	322	DC	Sidechain
2	F	413	DG	Sidechain
2	F	414	DG	Sidechain
2	F	419	DG	Sidechain
2	F	420	DC	Sidechain
2	F	424	DC	Sidechain
2	F	425	DC	Sidechain

## 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	E	672	0	380	95	0
2	F	675	0	377	65	0
3	A	944	0	962	41	0
3	B	944	0	962	54	0
3	C	944	0	962	57	0
3	D	944	0	962	49	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	5135	0	4605	333	0

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 35.

All (333) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:327:DT:H2''	1:E:328:DA:H5''	1.24	1.15
1:E:328:DA:H2''	1:E:329:DT:H5''	1.15	1.14
3:C:27:ARG:HG3	3:C:27:ARG:HH11	1.10	1.14
1:E:330:DT:H2''	1:E:331:DT:H5''	1.25	1.13
1:E:301:DA:H2''	1:E:302:DT:H5''	1.33	1.11
1:E:329:DT:H2''	1:E:330:DT:H5''	1.11	1.10
1:E:325:DA:H2''	1:E:326:DT:H5''	1.16	1.10
2:F:410:DT:H2''	2:F:411:DT:H5'	1.38	1.06
1:E:302:DT:O4	2:F:433:DA:N1	1.89	1.05
2:F:418:DA:H2''	2:F:419:DG:H5''	1.41	1.03
2:F:431:DA:H2''	2:F:432:DT:H5'	1.40	1.02
1:E:329:DT:C2'	1:E:330:DT:H5''	1.91	1.00
1:E:328:DA:C2'	1:E:329:DT:H5''	1.92	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:331:DT:H2''	1:E:332:DT:O4'	1.62	0.98
1:E:301:DA:C2'	1:E:302:DT:H5''	1.93	0.97
2:F:410:DT:H2'	2:F:411:DT:H71	1.43	0.96
1:E:307:DT:H2''	1:E:308:DT:H5'	1.49	0.94
1:E:327:DT:C2'	1:E:328:DA:H5''	1.97	0.94
1:E:325:DA:C2'	1:E:326:DT:H5''	1.98	0.93
1:E:330:DT:C2'	1:E:331:DT:H5''	2.00	0.92
2:F:404:DA:H2''	2:F:405:DA:N7	1.84	0.92
3:C:103:ARG:HB3	3:D:107:VAL:HG22	1.50	0.92
1:E:303:DA:H2''	1:E:304:DT:H5''	1.51	0.91
1:E:329:DT:H2''	1:E:330:DT:C5'	1.98	0.91
3:A:89:ILE:HG13	3:A:90:ILE:N	1.84	0.91
1:E:317:DT:H5'	1:E:317:DT:H6	1.36	0.90
1:E:325:DA:H2''	1:E:326:DT:C5'	2.03	0.89
2:F:431:DA:H2''	2:F:432:DT:C5'	2.03	0.89
2:F:405:DA:H2''	2:F:406:DA:H5''	1.55	0.88
3:C:27:ARG:HG3	3:C:27:ARG:NH1	1.81	0.88
2:F:404:DA:C2	2:F:405:DA:C2	2.62	0.87
1:E:307:DT:H2'	1:E:308:DT:H72	1.55	0.86
1:E:302:DT:H2''	1:E:303:DA:C8	2.10	0.86
3:A:103:ARG:HB3	3:B:107:VAL:HG22	1.56	0.86
2:F:430:DT:H2''	2:F:431:DA:H5''	1.57	0.86
2:F:404:DA:H2''	2:F:405:DA:C8	2.10	0.85
3:C:27:ARG:CG	3:C:27:ARG:HH11	1.89	0.84
2:F:406:DA:H2''	2:F:407:DT:H5'	1.61	0.83
2:F:418:DA:H2''	2:F:419:DG:C5'	2.10	0.82
3:D:12:LEU:HD13	3:D:48:MET:HE1	1.64	0.80
1:E:303:DA:C2'	1:E:304:DT:H5''	2.12	0.79
1:E:328:DA:H2''	1:E:329:DT:C5'	2.06	0.76
1:E:307:DT:H2'	1:E:308:DT:C7	2.16	0.75
2:F:410:DT:H2''	2:F:411:DT:C5'	2.15	0.75
3:D:28:ALA:O	3:D:32:GLU:HG3	1.86	0.75
1:E:302:DT:C2'	1:E:303:DA:C8	2.69	0.74
2:F:418:DA:C2'	2:F:419:DG:H5''	2.15	0.74
3:D:59:ASP:N	3:D:59:ASP:OD1	2.21	0.74
3:B:15:ILE:HG22	3:B:64:MET:HE3	1.68	0.73
2:F:410:DT:H5'	2:F:410:DT:H6	1.52	0.73
3:B:69:ARG:O	3:B:73:THR:HG23	1.88	0.73
3:D:4:LEU:O	3:D:6:ASP:N	2.21	0.73
3:A:37:SER:OG	3:A:39:PRO:HD2	1.88	0.73
1:E:330:DT:H2''	1:E:331:DT:C5'	2.11	0.73
1:E:315:DG:H2''	1:E:316:DC:H5'	1.70	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:301:DA:C3'	1:E:302:DT:H5''	2.20	0.72
3:A:89:ILE:HD13	3:B:89:ILE:HG21	1.72	0.72
2:F:401:DT:HO5'	2:F:401:DT:H6	1.36	0.72
3:C:83:GLU:O	3:C:87:THR:HB	1.89	0.71
2:F:422:DA:H2''	2:F:423:DT:H5'	1.72	0.71
2:F:405:DA:C2'	2:F:406:DA:H5''	2.21	0.71
1:E:301:DA:H2''	1:E:302:DT:C5'	2.17	0.70
1:E:310:DG:H1'	1:E:311:DG:H5''	1.73	0.70
1:E:324:DA:H2''	1:E:325:DA:H5''	1.73	0.69
1:E:327:DT:H2''	1:E:328:DA:C5'	2.15	0.69
1:E:306:DA:H2''	1:E:307:DT:H5''	1.75	0.69
1:E:315:DG:H2''	1:E:316:DC:C5'	2.23	0.69
1:E:327:DT:H2''	1:E:328:DA:H8	1.59	0.67
3:C:17:GLU:O	3:C:21:GLU:HG3	1.96	0.66
3:C:89:ILE:HG13	3:C:90:ILE:N	2.09	0.66
1:E:311:DG:H8	1:E:311:DG:H5'	1.60	0.65
3:C:29:ARG:HH12	3:C:32:GLU:CD	1.99	0.65
1:E:328:DA:C2	2:F:408:DA:C2	2.84	0.65
3:A:4:LEU:O	3:A:6:ASP:N	2.24	0.65
3:C:89:ILE:CD1	3:D:89:ILE:HG21	2.26	0.65
2:F:430:DT:C2'	2:F:431:DA:H5''	2.26	0.64
2:F:431:DA:H2'	2:F:432:DT:H72	1.79	0.64
3:D:69:ARG:O	3:D:73:THR:HG23	1.98	0.64
3:B:12:LEU:HD13	3:B:48:MET:HE1	1.79	0.64
3:C:89:ILE:HD12	3:D:89:ILE:HG21	1.80	0.64
3:D:37:SER:OG	3:D:39:PRO:HD2	1.98	0.63
1:E:331:DT:C2'	1:E:332:DT:O4'	2.42	0.63
3:C:37:SER:OG	3:C:39:PRO:HD2	1.99	0.63
2:F:423:DT:OP2	3:D:47:ARG:NH1	2.32	0.63
3:D:101:ALA:O	3:D:105:GLU:HG2	1.99	0.62
2:F:428:DA:H2''	2:F:429:DT:OP2	2.00	0.62
3:C:30:ILE:CG2	3:C:34:LEU:HD12	2.29	0.62
3:A:109:SER:HB3	3:B:100:GLU:OE2	1.99	0.62
3:B:85:LEU:HD22	3:B:116:LEU:HD21	1.81	0.62
1:E:314:DA:H2''	1:E:315:DG:H5'	1.82	0.61
2:F:432:DT:H2''	2:F:433:DA:C8	2.35	0.61
3:B:4:LEU:O	3:B:6:ASP:N	2.32	0.61
1:E:327:DT:C3'	1:E:328:DA:H5''	2.30	0.60
3:D:41:VAL:O	3:D:45:VAL:HG23	2.01	0.60
3:C:83:GLU:HG2	3:C:97:VAL:HG12	1.83	0.60
3:C:4:LEU:C	3:C:6:ASP:H	2.04	0.60
1:E:302:DT:H3	2:F:433:DA:H2	1.49	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:84:ARG:HB3	3:C:120:LEU:HD13	1.81	0.60
3:B:59:ASP:N	3:B:59:ASP:OD1	2.25	0.60
1:E:331:DT:H3	2:F:404:DA:H61	1.50	0.60
3:D:44:THR:O	3:D:48:MET:HG3	2.00	0.60
3:C:109:SER:HB3	3:D:100:GLU:OE2	2.01	0.60
1:E:317:DT:H2''	1:E:318:DT:C6	2.38	0.59
3:C:113:GLU:O	3:C:117:VAL:HG12	2.03	0.58
1:E:328:DA:C3'	1:E:329:DT:H5''	2.33	0.58
1:E:331:DT:H2''	1:E:332:DT:H5''	1.86	0.58
1:E:317:DT:H5'	1:E:317:DT:C6	2.28	0.58
1:E:303:DA:C3'	1:E:304:DT:H5''	2.34	0.58
3:D:83:GLU:HG2	3:D:97:VAL:HG12	1.85	0.58
1:E:309:DA:C2	2:F:427:DA:C2	2.92	0.58
3:B:65:THR:HB	3:B:66:PRO:HD2	1.86	0.58
3:A:4:LEU:C	3:A:6:ASP:H	2.06	0.57
3:B:41:VAL:O	3:B:45:VAL:HG23	2.03	0.57
1:E:306:DA:H2''	1:E:307:DT:C5'	2.33	0.57
1:E:325:DA:H2'	1:E:326:DT:H71	1.85	0.57
1:E:313:DT:H2''	1:E:314:DA:C8	2.39	0.57
1:E:307:DT:C6	1:E:308:DT:H72	2.40	0.57
3:D:58:SER:C	3:D:60:ARG:H	2.08	0.57
1:E:306:DA:C2'	1:E:307:DT:H5''	2.34	0.56
3:B:29:ARG:HH12	3:B:32:GLU:CD	2.08	0.56
1:E:301:DA:H8	1:E:301:DA:HO5'	1.51	0.56
1:E:330:DT:C3'	1:E:331:DT:H5''	2.36	0.56
3:A:28:ALA:O	3:A:32:GLU:HG3	2.04	0.56
1:E:326:DT:H2'	1:E:327:DT:H72	1.87	0.56
2:F:426:DT:H2''	2:F:427:DA:H5''	1.87	0.56
3:D:57:ALA:HB2	3:D:63:GLN:HG3	1.88	0.56
1:E:324:DA:C2'	1:E:325:DA:H5''	2.36	0.56
3:A:84:ARG:HB3	3:A:120:LEU:HD13	1.87	0.56
2:F:423:DT:H2''	2:F:424:DC:H5''	1.88	0.56
3:B:28:ALA:O	3:B:32:GLU:HG2	2.05	0.56
1:E:323:DT:H71	3:B:39:PRO:HG2	1.88	0.55
3:A:101:ALA:O	3:A:105:GLU:HG2	2.06	0.55
3:B:44:THR:O	3:B:48:MET:HG3	2.06	0.55
3:A:18:LEU:HD21	3:A:29:ARG:HB2	1.88	0.55
2:F:404:DA:C2'	2:F:405:DA:N7	2.64	0.55
3:A:103:ARG:HB2	3:A:103:ARG:HH11	1.71	0.55
1:E:307:DT:H6	1:E:307:DT:H5'	1.71	0.54
1:E:331:DT:H2''	1:E:332:DT:C6	2.42	0.54
1:E:310:DG:C2'	1:E:311:DG:H5''	2.37	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:92:LEU:HG	3:A:93:ASP:N	2.21	0.54
3:C:112:VAL:HG13	3:D:90:ILE:HG21	1.89	0.54
3:D:84:ARG:NH2	3:D:88:ASP:OD2	2.41	0.54
3:A:43:GLN:O	3:A:46:ALA:HB3	2.08	0.54
3:A:107:VAL:O	3:B:103:ARG:NH1	2.40	0.54
2:F:404:DA:C4	2:F:405:DA:C6	2.95	0.54
2:F:432:DT:H2''	2:F:433:DA:H8	1.72	0.54
3:A:16:TYR:CE2	3:A:76:MET:HG2	2.42	0.54
3:C:86:LEU:HD23	3:C:90:ILE:HD12	1.89	0.54
3:C:103:ARG:HB3	3:D:107:VAL:CG2	2.29	0.53
3:A:89:ILE:CD1	3:B:89:ILE:HG21	2.37	0.53
1:E:311:DG:C8	1:E:311:DG:H5'	2.42	0.53
3:C:105:GLU:HG3	3:C:106:HIS:CD2	2.43	0.53
3:D:116:LEU:HG	3:D:120:LEU:HD22	1.89	0.53
1:E:327:DT:H2''	1:E:328:DA:C8	2.42	0.53
3:B:101:ALA:O	3:B:105:GLU:HG2	2.09	0.53
3:C:92:LEU:HG	3:C:93:ASP:N	2.23	0.53
1:E:302:DT:H2'	1:E:303:DA:C8	2.44	0.52
2:F:429:DT:H1'	2:F:430:DT:H5''	1.92	0.52
3:C:82:ALA:O	3:C:86:LEU:HG	2.09	0.52
2:F:410:DT:C2'	2:F:411:DT:H71	2.31	0.52
2:F:420:DC:H2''	2:F:421:DT:H71	1.92	0.51
1:E:331:DT:C2'	1:E:332:DT:C6	2.94	0.51
1:E:303:DA:H2''	1:E:304:DT:C6	2.46	0.51
3:D:12:LEU:CD1	3:D:48:MET:HE1	2.39	0.51
3:A:83:GLU:O	3:A:87:THR:HB	2.10	0.51
3:C:23:VAL:HG12	3:C:24:THR:N	2.26	0.51
3:C:93:ASP:HB3	3:C:96:LYS:HD3	1.93	0.51
1:E:326:DT:H2'	1:E:327:DT:C7	2.40	0.51
3:C:4:LEU:O	3:C:6:ASP:N	2.35	0.51
2:F:401:DT:O5'	2:F:401:DT:H6	1.93	0.51
3:C:18:LEU:HD21	3:C:29:ARG:HB2	1.92	0.51
3:B:11:TYR:CE1	3:B:34:LEU:HD12	2.45	0.50
2:F:404:DA:C4	2:F:405:DA:C5	2.99	0.50
3:A:103:ARG:HB3	3:B:107:VAL:CG2	2.34	0.50
3:C:13:ARG:NH1	3:C:79:HIS:ND1	2.59	0.50
3:B:50:ARG:C	3:B:52:GLY:H	2.15	0.50
2:F:405:DA:C3'	2:F:406:DA:H5''	2.42	0.50
3:A:85:LEU:HD22	3:A:89:ILE:HG12	1.94	0.50
3:D:82:ALA:O	3:D:86:LEU:HD12	2.12	0.50
3:A:115:ARG:O	3:A:118:LYS:N	2.44	0.50
3:A:103:ARG:CB	3:A:103:ARG:HH11	2.24	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:116:LEU:O	3:D:120:LEU:HB2	2.12	0.50
3:C:90:ILE:O	3:D:115:ARG:HD2	2.12	0.49
3:D:94:ILE:O	3:D:94:ILE:HD13	2.12	0.49
1:E:305:DA:H1'	1:E:306:DA:H5''	1.94	0.49
2:F:431:DA:H2'	2:F:432:DT:C7	2.41	0.49
2:F:417:DA:H2''	2:F:418:DA:C5'	2.42	0.49
1:E:326:DT:C6	1:E:327:DT:H72	2.47	0.49
3:C:108:MET:HE1	3:C:113:GLU:HA	1.94	0.49
3:C:16:TYR:CE1	3:C:76:MET:HG2	2.48	0.49
3:D:15:ILE:HG22	3:D:64:MET:HE3	1.94	0.49
2:F:409:DA:H2''	2:F:410:DT:H5''	1.95	0.49
2:F:404:DA:N3	2:F:405:DA:C4	2.80	0.49
1:E:317:DT:H2'	1:E:318:DT:H71	1.95	0.49
3:C:30:ILE:HG23	3:C:34:LEU:HD12	1.95	0.49
3:B:59:ASP:O	3:B:60:ARG:HB2	2.13	0.49
3:A:4:LEU:C	3:A:6:ASP:N	2.66	0.49
3:B:112:VAL:O	3:B:116:LEU:HB2	2.13	0.48
1:E:307:DT:H2''	1:E:308:DT:C5'	2.32	0.48
3:C:114:ARG:O	3:C:117:VAL:HG13	2.13	0.48
3:C:31:ALA:HB2	3:C:41:VAL:HG21	1.94	0.48
3:B:26:LEU:O	3:B:29:ARG:N	2.41	0.48
2:F:425:DC:C2'	2:F:426:DT:H72	2.43	0.48
3:B:94:ILE:HD13	3:B:94:ILE:O	2.14	0.48
2:F:431:DA:H2''	2:F:432:DT:H5''	1.91	0.48
1:E:310:DG:H2''	1:E:311:DG:H5''	1.93	0.48
3:B:105:GLU:HG3	3:B:106:HIS:CD2	2.49	0.48
1:E:319:DT:H1'	1:E:320:DA:H5'	1.94	0.48
1:E:331:DT:C2'	1:E:332:DT:H5''	2.44	0.47
3:D:79:HIS:CE1	3:D:98:HIS:CE1	3.02	0.47
3:D:17:GLU:O	3:D:21:GLU:HG2	2.15	0.47
3:C:41:VAL:O	3:C:45:VAL:HG23	2.14	0.47
3:C:76:MET:O	3:C:79:HIS:HB3	2.15	0.47
2:F:410:DT:H5'	2:F:410:DT:C6	2.42	0.47
3:A:113:GLU:O	3:A:117:VAL:HG12	2.14	0.47
2:F:408:DA:H1'	2:F:409:DA:H5''	1.97	0.47
2:F:430:DT:C2	2:F:431:DA:C8	3.03	0.47
3:B:38:GLY:N	3:B:39:PRO:HD2	2.30	0.47
3:A:85:LEU:HG	3:A:116:LEU:HD11	1.97	0.47
3:D:92:LEU:HG	3:D:93:ASP:N	2.30	0.47
3:D:10:MET:SD	3:D:106:HIS:CE1	3.08	0.46
3:A:112:VAL:HG13	3:B:90:ILE:HG21	1.98	0.46
2:F:413:DG:H2''	2:F:414:DG:H5''	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:58:SER:C	3:B:60:ARG:H	2.17	0.46
3:B:79:HIS:HB2	3:B:105:GLU:OE1	2.15	0.46
2:F:410:DT:C5'	2:F:410:DT:H6	2.26	0.46
1:E:323:DT:H71	3:B:39:PRO:CG	2.46	0.46
1:E:327:DT:C2	1:E:328:DA:C8	3.04	0.46
3:C:43:GLN:O	3:C:46:ALA:HB3	2.16	0.46
3:C:59:ASP:OD1	3:C:59:ASP:N	2.49	0.46
3:B:84:ARG:HG2	3:B:84:ARG:HH11	1.80	0.46
1:E:312:DA:H2''	1:E:313:DT:H5'	1.97	0.46
3:A:89:ILE:CG1	3:A:90:ILE:N	2.69	0.46
3:A:31:ALA:HB2	3:A:41:VAL:HG21	1.98	0.46
2:F:404:DA:C2'	2:F:405:DA:C8	2.94	0.45
2:F:425:DC:H2'	2:F:426:DT:H72	1.97	0.45
1:E:314:DA:H2''	1:E:315:DG:C5'	2.45	0.45
3:A:18:LEU:HA	3:A:18:LEU:HD12	1.86	0.45
3:B:116:LEU:O	3:B:120:LEU:HB2	2.16	0.45
2:F:432:DT:C2'	2:F:433:DA:C8	2.99	0.45
3:D:100:GLU:OE1	3:D:104:TRP:NE1	2.50	0.45
3:C:69:ARG:O	3:C:72:ALA:HB3	2.16	0.45
3:C:116:LEU:HA	3:C:119:VAL:HG22	1.98	0.45
1:E:321:DC:H2'	3:B:40:THR:CG2	2.46	0.45
3:B:118:LYS:O	3:B:119:VAL:C	2.56	0.44
1:E:301:DA:H2''	1:E:302:DT:O4'	2.17	0.44
3:A:103:ARG:NH1	3:B:107:VAL:O	2.50	0.44
3:C:37:SER:O	3:C:41:VAL:HG23	2.16	0.44
1:E:303:DA:H2''	1:E:304:DT:O4'	2.18	0.44
3:D:85:LEU:HD22	3:D:116:LEU:HD21	1.99	0.44
3:A:29:ARG:HH12	3:A:32:GLU:CD	2.21	0.44
1:E:313:DT:H2''	1:E:314:DA:H8	1.83	0.44
3:A:74:ALA:O	3:A:78:LYS:HG3	2.18	0.44
3:B:85:LEU:N	3:B:120:LEU:HD21	2.32	0.44
3:B:74:ALA:O	3:B:78:LYS:HG3	2.18	0.44
3:B:13:ARG:HH12	3:B:79:HIS:CE1	2.36	0.43
3:C:115:ARG:O	3:C:118:LYS:N	2.51	0.43
3:B:12:LEU:HD13	3:B:48:MET:CE	2.47	0.43
2:F:417:DA:C2'	2:F:418:DA:H5''	2.48	0.43
3:B:100:GLU:OE1	3:B:104:TRP:NE1	2.51	0.43
3:C:89:ILE:CG1	3:C:90:ILE:N	2.78	0.43
3:B:116:LEU:HA	3:B:116:LEU:HD12	1.89	0.43
3:B:27:ARG:HG2	3:B:45:VAL:HG21	2.00	0.43
3:D:43:GLN:HG2	3:D:47:ARG:HH21	1.84	0.43
1:E:331:DT:C2	1:E:332:DT:C2	3.06	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:29:ARG:NH1	3:C:32:GLU:CD	2.70	0.43
3:A:71:LEU:HD23	3:A:71:LEU:H	1.84	0.43
3:D:4:LEU:HD21	3:D:34:LEU:CD1	2.49	0.43
3:B:71:LEU:O	3:B:74:ALA:N	2.52	0.43
3:B:56:VAL:HG22	3:B:62:LEU:HD12	2.00	0.43
3:C:7:THR:O	3:C:8:THR:C	2.57	0.43
3:C:4:LEU:C	3:C:6:ASP:N	2.69	0.43
1:E:310:DG:C1'	1:E:311:DG:H5''	2.44	0.43
3:D:111:GLU:HA	3:D:111:GLU:OE1	2.18	0.42
3:C:108:MET:HE2	3:C:108:MET:HB3	1.90	0.42
1:E:319:DT:H2''	1:E:320:DA:O5'	2.19	0.42
1:E:329:DT:C3'	1:E:330:DT:H5''	2.42	0.42
3:A:89:ILE:HD12	3:B:89:ILE:HD13	2.00	0.42
3:D:50:ARG:C	3:D:52:GLY:H	2.23	0.42
3:C:104:TRP:CD1	3:D:107:VAL:HG13	2.55	0.42
3:D:58:SER:C	3:D:60:ARG:N	2.71	0.42
1:E:332:DT:H2''	1:E:333:DA:C8	2.55	0.42
2:F:431:DA:C2'	2:F:432:DT:C5'	2.86	0.42
3:D:95:ASN:HD22	3:D:95:ASN:H	1.67	0.42
1:E:332:DT:C2'	1:E:333:DA:C8	3.02	0.42
2:F:428:DA:C8	2:F:429:DT:C7	3.02	0.42
2:F:427:DA:H2''	2:F:428:DA:C8	2.55	0.41
1:E:307:DT:C2'	1:E:308:DT:C7	2.94	0.41
3:C:109:SER:CB	3:D:100:GLU:OE2	2.67	0.41
2:F:404:DA:C2	2:F:405:DA:N3	2.88	0.41
2:F:417:DA:H2''	2:F:418:DA:H5''	2.02	0.41
2:F:422:DA:H2''	2:F:423:DT:C5'	2.48	0.41
3:D:87:THR:O	3:D:91:GLY:HA2	2.20	0.41
2:F:413:DG:C2'	2:F:414:DG:H5''	2.50	0.41
3:A:86:LEU:CD1	3:A:100:GLU:HB3	2.50	0.41
1:E:331:DT:C3'	1:E:332:DT:H5''	2.51	0.41
1:E:330:DT:H2''	1:E:331:DT:O4'	2.20	0.41
3:D:26:LEU:O	3:D:29:ARG:HB2	2.20	0.41
1:E:310:DG:H2''	1:E:311:DG:C5'	2.51	0.41
3:C:54:VAL:HG22	3:C:55:VAL:H	1.86	0.41
3:C:104:TRP:CD1	3:C:104:TRP:N	2.89	0.41
3:D:29:ARG:NH1	3:D:32:GLU:OE1	2.51	0.41
2:F:423:DT:C2'	2:F:424:DC:H5''	2.49	0.41
3:C:85:LEU:HD22	3:C:89:ILE:HG12	2.03	0.41
3:C:110:ASP:O	3:C:113:GLU:HB3	2.21	0.41
3:B:10:MET:SD	3:B:106:HIS:CE1	3.13	0.41
3:D:86:LEU:O	3:D:91:GLY:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:414:DG:OP2	3:C:28:ALA:HB2	2.20	0.41
3:B:93:ASP:CG	3:B:95:ASN:HD22	2.24	0.41
1:E:303:DA:H2''	1:E:304:DT:C5'	2.37	0.41
3:C:87:THR:HG22	3:C:88:ASP:N	2.35	0.41
3:B:50:ARG:C	3:B:52:GLY:N	2.74	0.41
3:B:83:GLU:HG2	3:B:97:VAL:HG12	2.03	0.41
3:A:17:GLU:O	3:A:21:GLU:HG3	2.21	0.41
1:E:307:DT:H2''	1:E:308:DT:C6	2.55	0.41
2:F:429:DT:H2''	2:F:430:DT:OP2	2.21	0.41
2:F:420:DC:C2'	2:F:421:DT:H71	2.51	0.41
3:A:87:THR:HG22	3:A:88:ASP:N	2.36	0.41
3:D:12:LEU:HD12	3:D:12:LEU:HA	1.78	0.40
3:D:29:ARG:HD3	3:D:29:ARG:HA	1.65	0.40
3:A:29:ARG:NH1	3:A:32:GLU:CD	2.75	0.40
3:A:108:MET:HE1	3:A:113:GLU:HA	2.03	0.40
3:B:29:ARG:NH1	3:B:32:GLU:CD	2.75	0.40
1:E:327:DT:C2'	1:E:328:DA:C8	3.05	0.40
3:A:82:ALA:O	3:A:86:LEU:HG	2.21	0.40
3:B:16:TYR:HB2	3:B:64:MET:HE1	2.04	0.40
3:B:71:LEU:O	3:B:72:ALA:C	2.59	0.40
3:A:69:ARG:O	3:A:72:ALA:HB3	2.22	0.40
3:D:84:ARG:HH11	3:D:84:ARG:HG2	1.85	0.40
3:D:85:LEU:N	3:D:120:LEU:HD21	2.37	0.40
3:C:13:ARG:HH12	3:C:79:HIS:CE1	2.40	0.40
3:B:92:LEU:HG	3:B:93:ASP:N	2.36	0.40
3:C:111:GLU:OE1	3:C:111:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

## 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	
3	A	116/226 (51%)	102 (88%)	13 (11%)	1 (1%)	25	73
3	B	116/226 (51%)	102 (88%)	13 (11%)	1 (1%)	25	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	116/226 (51%)	104 (90%)	11 (10%)	1 (1%)	25	73
3	D	116/226 (51%)	104 (90%)	10 (9%)	2 (2%)	14	54
All	All	464/904 (51%)	412 (89%)	47 (10%)	5 (1%)	21	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	5	VAL
3	B	119	VAL
3	C	5	VAL
3	A	5	VAL
3	D	119	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	
3	A	105/198 (53%)	87 (83%)	18 (17%)	3	15
3	B	105/198 (53%)	86 (82%)	19 (18%)	2	13
3	C	105/198 (53%)	87 (83%)	18 (17%)	3	15
3	D	105/198 (53%)	87 (83%)	18 (17%)	3	15
All	All	420/792 (53%)	347 (83%)	73 (17%)	3	14

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	4	LEU
3	A	18	LEU
3	A	29	ARG
3	A	35	GLU
3	A	37	SER
3	A	54	VAL
3	A	58	SER
3	A	71	LEU
3	A	85	LEU

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Mol	Chain	Res	Type
3	A	87	THR
3	A	89	ILE
3	A	92	LEU
3	A	94	ILE
3	A	103	ARG
3	A	108	MET
3	A	114	ARG
3	A	116	LEU
3	A	117	VAL
3	B	12	LEU
3	B	20	GLU
3	B	26	LEU
3	B	29	ARG
3	B	32	GLU
3	B	37	SER
3	B	47	ARG
3	B	54	VAL
3	B	58	SER
3	B	59	ASP
3	B	62	LEU
3	B	67	THR
3	B	81	LEU
3	B	94	ILE
3	B	107	VAL
3	B	111	GLU
3	B	114	ARG
3	B	117	VAL
3	B	120	LEU
3	C	4	LEU
3	C	18	LEU
3	C	27	ARG
3	C	29	ARG
3	C	58	SER
3	C	60	ARG
3	C	71	LEU
3	C	84	ARG
3	C	85	LEU
3	C	87	THR
3	C	89	ILE
3	C	94	ILE
3	C	96	LYS
3	C	108	MET

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Mol	Chain	Res	Type
3	C	111	GLU
3	C	116	LEU
3	C	117	VAL
3	C	118	LYS
3	D	12	LEU
3	D	20	GLU
3	D	29	ARG
3	D	34	LEU
3	D	37	SER
3	D	54	VAL
3	D	59	ASP
3	D	62	LEU
3	D	67	THR
3	D	71	LEU
3	D	94	ILE
3	D	105	GLU
3	D	107	VAL
3	D	111	GLU
3	D	114	ARG
3	D	115	ARG
3	D	117	VAL
3	D	120	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	95	ASN
3	D	95	ASN

### 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 8 ligands modelled in this entry, 8 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.

## 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.