



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:35 PM UTC

PDB ID : 4G83 / pdb_00004g83
Title : Crystal Structure of p73 DNA-Binding Domain Tetramer bound to a Full Response-Element
Authors : Ethayathulla, A.S.; Viadiu, H.
Deposited on : 2012-07-20
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	:	4-5-2 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

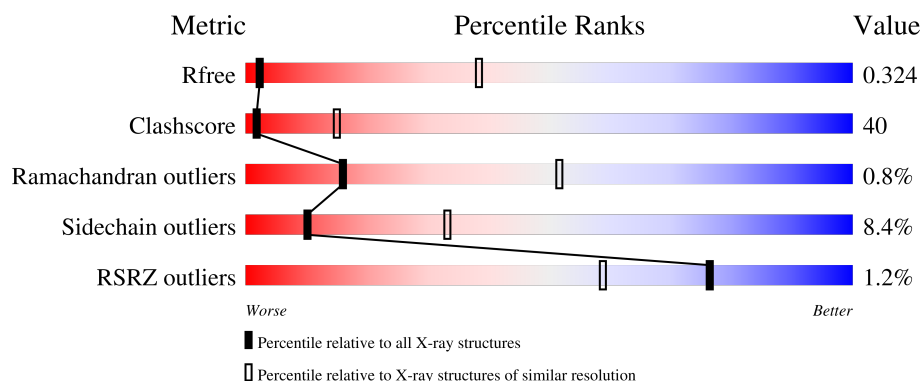
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	E	20	
1	F	20	
2	A	210	
2	B	210	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3506 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 DNA chain called dna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	10	Total	C	N	O	P	0	0	0
			205	97	38	60	10			
1	F	10	Total	C	N	O	P	0	0	0
			205	97	38	60	10			

- Molecule 2 is a protein called Tumor protein p73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	198	Total	C	N	O	S	1	0	0
			1547	969	279	288	11			
2	B	198	Total	C	N	O	S	2	0	0
			1547	969	279	288	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	expression tag	UNP O15350
A	104	GLY	-	expression tag	UNP O15350
A	105	HIS	-	expression tag	UNP O15350
A	106	HIS	-	expression tag	UNP O15350
A	107	HIS	-	expression tag	UNP O15350
A	108	HIS	-	expression tag	UNP O15350
A	109	HIS	-	expression tag	UNP O15350
A	110	HIS	-	expression tag	UNP O15350
A	111	HIS	-	expression tag	UNP O15350
A	112	HIS	-	expression tag	UNP O15350
A	113	GLU	-	expression tag	UNP O15350
A	114	PHE	-	expression tag	UNP O15350
B	103	MET	-	expression tag	UNP O15350
B	104	GLY	-	expression tag	UNP O15350
B	105	HIS	-	expression tag	UNP O15350
B	106	HIS	-	expression tag	UNP O15350
B	107	HIS	-	expression tag	UNP O15350

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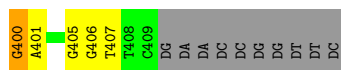
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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	HIS	-	expression tag	UNP O15350
B	109	HIS	-	expression tag	UNP O15350
B	110	HIS	-	expression tag	UNP O15350
B	111	HIS	-	expression tag	UNP O15350
B	112	HIS	-	expression tag	UNP O15350
B	113	GLU	-	expression tag	UNP O15350
B	114	PHE	-	expression tag	UNP O15350

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0

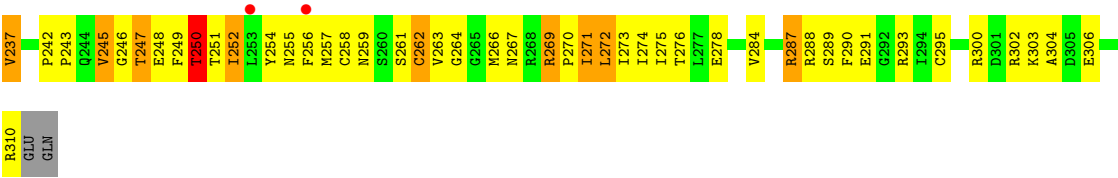
- Molecule 1: dna



G410	G416	T417	T418	C419	DG	DA	DA	DC	DC	DG	DG	DT	DT	DC
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T247	T248	T249	T250	T251	T252	T253	T254	M257	M258	M259	M260	M261	M262	M263	M264	M265	M266	M267	M268	M269	M270	M271	M272	M273	M274	M275	M276	M277	M278	M279	M280	M281	M282	M283	M284	M285	M286	M287	M288	M289	M290	M291	M292	M293	M294	M295	M296	M297	M298	M299	M300	M301	M302	M303	M304	M305	M306	M307	M308	M309	M310	M311	M312	M313	M314	M315	M316	M317	M318	M319	M320	M321	M322	M323	M324	M325	M326	M327	M328	M329	M330	M331	M332	M333	M334	M335	M336	M337	M338	M339	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353	M354	M355	M356	M357	M358	M359	M360	M361	M362	M363	M364	M365	M366	M367	M368	M369	M370	M371	M372	M373	M374	M375	M376	M377	M378	M379	M380	M381	M382	M383	M384	M385	M386	M387	M388	M389	M390	M391	M392	M393	M394	M395	M396	M397	M398	M399	M400	M401	M402	M403	M404	M405	M406	M407	M408	M409	M410	M411	M412	M413	M414	M415	M416	M417	M418	M419	M420	M421	M422	M423	M424	M425	M426	M427	M428	M429	M430	M431	M432	M433	M434	M435	M436	M437	M438	M439	M440	M441	M442	M443	M444	M445	M446	M447	M448	M449	M450	M451	M452	M453	M454	M455	M456	M457	M458	M459	M460	M461	M462	M463	M464	M465	M466	M467	M468	M469	M470	M471	M472	M473	M474	M475	M476	M477	M478	M479	M480	M481	M482	M483	M484	M485	M486	M487	M488	M489	M490	M491	M492	M493	M494	M495	M496	M497	M498	M499	M500	M501	M502	M503	M504	M505	M506	M507	M508	M509	M510	M511	M512	M513	M514	M515	M516	M517	M518	M519	M520	M521	M522	M523	M524	M525	M526	M527	M528	M529	M530	M531	M532	M533	M534	M535	M536	M537	M538	M539	M540	M541	M542	M543	M544	M545	M546	M547	M548	M549	M550	M551	M552	M553	M554	M555	M556	M557	M558	M559	M560	M561	M562	M563	M564	M565	M566	M567	M568	M569	M570	M571	M572	M573	M574	M575	M576	M577	M578	M579	M580	M581	M582	M583	M584	M585	M586	M587	M588	M589	M590	M591	M592	M593	M594	M595	M596	M597	M598	M599	M600	M601	M602	M603	M604	M605	M606	M607	M608	M609	M610	M611	M612	M613	M614	M615	M616	M617	M618	M619	M620	M621	M622	M623	M624	M625	M626	M627	M628	M629	M630	M631	M632	M633	M634	M635	M636	M637	M638	M639	M640	M641	M642	M643	M644	M645	M646	M647	M648	M649	M650	M651	M652	M653	M654	M655	M656	M657	M658	M659	M660	M661	M662	M663	M664	M665	M666	M667	M668	M669	M670	M671	M672	M673	M674	M675	M676	M677	M678	M679	M680	M681	M682	M683	M684	M685	M686	M687	M688	M689	M690	M691	M692	M693	M694	M695	M696	M697	M698	M699	M700	M701	M702	M703	M704	M705	M706	M707	M708	M709	M710	M711	M712	M713	M714	M715	M716	M717	M718	M719	M720	M721	M722	M723	M724	M725	M726	M727	M728	M729	M730	M731	M732	M733	M734	M735	M736	M737	M738	M739	M740	M741	M742	M743	M744	M745	M746	M747	M748	M749	M750	M751	M752	M753	M754	M755	M756	M757	M758	M759	M76
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AlT4	AlT5	AlT6	AlT7	AlT8	AlT9	AlT10	AlT11	AlT12	AlT13	AlT14	AlT15	AlT16	AlT17	AlT18	AlT19	AlT20	AlT21	AlT22	AlT23	AlT24	AlT25	AlT26	AlT27	AlT28	AlT29	AlT30	AlT31	AlT32	AlT33	AlT34	AlT35	AlT36	AlT37	AlT38	AlT39	AlT40	AlT41	AlT42	AlT43	AlT44	AlT45	AlT46	AlT47	AlT48	AlT49	AlT50	AlT51	AlT52	AlT53	AlT54	AlT55	AlT56	AlT57	AlT58	AlT59	AlT60	AlT61	AlT62	AlT63	AlT64	AlT65	AlT66	AlT67	AlT68	AlT69	AlT70	AlT71	AlT72	AlT73	AlT74	AlT75	AlT76	AlT77	AlT78	AlT79	AlT80	AlT81	AlT82	AlT83	AlT84	AlT85	AlT86	AlT87	AlT88	AlT89	AlT90	AlT91	AlT92	AlT93	AlT94	AlT95	AlT96	AlT97	AlT98	AlT99	AlT100	AlT101	AlT102	AlT103	AlT104	AlT105	AlT106	AlT107	AlT108	AlT109	AlT110	AlT111	AlT112	AlT113	AlT114	AlT115	AlT116	AlT117	AlT118	AlT119	AlT120	AlT121	AlT122	AlT123	AlT124	AlT125	AlT126	AlT127	AlT128	AlT129	AlT130	AlT131	AlT132	AlT133	AlT134	AlT135	AlT136	AlT137	AlT138	AlT139	AlT140	AlT141	AlT142	AlT143	AlT144	AlT145	AlT146	AlT147	AlT148	AlT149	AlT150	AlT151	AlT152	AlT153	AlT154	AlT155	AlT156	AlT157	AlT158	AlT159	AlT160	AlT161	AlT162	AlT163	AlT164	AlT165	AlT166	AlT167	AlT168	AlT169	AlT170	AlT171	AlT172	AlT173	AlT174	AlT175	AlT176	AlT177	AlT178	AlT179	AlT180	AlT181	AlT182	AlT183	AlT184	AlT185	AlT186	AlT187	AlT188	AlT189	AlT190	AlT191	AlT192	AlT193	AlT194	AlT195	AlT196	AlT197	AlT198	AlT199	AlT200	AlT201	AlT202	AlT203	AlT204	AlT205	AlT206	AlT207	AlT208	AlT209	AlT210	AlT211	AlT212	AlT213	AlT214	AlT215	AlT216	AlT217	AlT218	AlT219	AlT220	AlT221	AlT222	AlT223	AlT224	AlT225	AlT226	AlT227	AlT228	AlT229	AlT230	AlT231	AlT232	AlT233	AlT234	AlT235	AlT236	AlT237	AlT238	AlT239	AlT240	AlT241	AlT242	AlT243	AlT244	AlT245	AlT246	AlT247	AlT248	AlT249	AlT250	AlT251	AlT252	AlT253	AlT254	AlT255	AlT256	AlT257	AlT258	AlT259	AlT260	AlT261	AlT262	AlT263	AlT264	AlT265	AlT266	AlT267	AlT268	AlT269	AlT270	AlT271	AlT272	AlT273	AlT274	AlT275	AlT276	AlT277	AlT278	AlT279	AlT280	AlT281	AlT282	AlT283	AlT284	AlT285	AlT286	AlT287	AlT288	AlT289	AlT290	AlT291	AlT292	AlT293	AlT294	AlT295	AlT296	AlT297	AlT298	AlT299	AlT300	AlT301	AlT302	AlT303	AlT304	AlT305	AlT306	AlT307	AlT308	AlT309	AlT310	AlT311	AlT312	AlT313	AlT314	AlT315	AlT316	AlT317	AlT318	AlT319	AlT320	AlT321	AlT322	AlT323	AlT324	AlT325	AlT326	AlT327	AlT328	AlT329	AlT330	AlT331	AlT332	AlT333	AlT334	AlT335	AlT336	AlT337	AlT338	AlT339	AlT340	AlT341	AlT342	AlT343	AlT344	AlT345	AlT346	AlT347	AlT348	AlT349	AlT350	AlT351	AlT352	AlT353	AlT354	AlT355	AlT356	AlT357	AlT358	AlT359	AlT360	AlT361	AlT362	AlT363	AlT364	AlT365	AlT366	AlT367	AlT368	AlT369	AlT370	AlT371	AlT372	AlT373	AlT374	AlT375	AlT376	AlT377	AlT378	AlT379	AlT380	AlT381	AlT382	AlT383	AlT384	AlT385	AlT386	AlT387	AlT388	AlT389	AlT390	AlT391	AlT392	AlT393	AlT394	AlT395	AlT396	AlT397	AlT398	AlT399	AlT400	AlT401	AlT402	AlT403	AlT404	AlT405	AlT406	AlT407	AlT408	AlT409	AlT410	AlT411	AlT412	AlT413	AlT414	AlT415	AlT416	AlT417	AlT418	AlT419	AlT420	AlT421	AlT422	AlT
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.72Å 96.34Å 34.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.61 – 4.00 45.61 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.61-4.00) 99.7 (45.61-4.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168, REFMAC 5.6.0117	Depositor
R, R_{free}	0.241 , 0.307 0.251 , 0.324	Depositor DCC
R_{free} test set	202 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 95.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3506	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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:
ZN

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	0.35	0/229	1.09	2/351 (0.6%)
1	F	0.27	0/229	1.04	0/351
2	A	0.76	1/1586 (0.1%)	1.63	41/2157 (1.9%)
2	B	0.92	2/1586 (0.1%)	2.14	55/2157 (2.5%)
All	All	0.80	3/3630 (0.1%)	1.81	98/5016 (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
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	167	THR	CA-CB	8.02	1.64	1.54
2	B	195	PRO	CA-C	5.79	1.61	1.52
2	B	196	ASN	N-CA	5.10	1.52	1.46

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	PRO	CA-C-N	-24.92	94.71	120.38
2	B	169	PRO	C-N-CA	-24.92	94.71	120.38
2	B	167	THR	CA-C-N	19.47	140.43	120.38
2	B	167	THR	C-N-CA	19.47	140.43	120.38
2	B	169	PRO	N-CA-C	14.54	128.44	110.70
2	B	198	GLU	N-CA-C	-13.54	96.52	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	170	PRO	CA-C-N	13.32	133.48	119.76
2	B	170	PRO	C-N-CA	13.32	133.48	119.76
2	B	185	GLU	N-CA-C	13.16	128.80	113.01
2	B	246	GLY	N-CA-C	12.82	133.12	115.30
2	B	242	PRO	CA-C-N	-12.80	107.36	120.03
2	B	242	PRO	C-N-CA	-12.80	107.36	120.03
2	B	196	ASN	N-CA-C	12.78	125.29	111.36
2	B	206	GLY	N-CA-C	10.13	124.75	112.49
2	B	187	VAL	N-CA-C	-9.78	98.83	111.05
2	B	168	PRO	N-CA-C	9.68	122.51	110.70
2	B	197	HIS	N-CA-C	9.56	121.78	111.36
2	A	242	PRO	CA-C-N	-9.47	109.79	119.92
2	A	242	PRO	C-N-CA	-9.47	109.79	119.92
2	A	137	ALA	N-CA-C	-8.78	97.49	110.48
2	B	250	THR	N-CA-C	-8.61	93.72	107.93
2	A	230	VAL	N-CA-C	8.58	119.14	110.82
2	A	200	GLY	N-CA-C	8.51	126.45	112.66
2	A	248	GLU	N-CA-C	-8.31	102.73	113.12
2	A	282	GLY	N-CA-C	8.31	124.58	114.69
2	B	168	PRO	CA-C-N	-8.27	111.86	120.38
2	B	168	PRO	C-N-CA	-8.27	111.86	120.38
2	A	115	ILE	N-CA-C	8.23	116.41	107.60
2	B	115	ILE	N-CA-C	7.96	116.81	107.73
2	B	202	ASP	N-CA-C	7.90	121.86	111.75
2	B	304	ALA	N-CA-C	7.85	119.62	111.14
2	B	195	PRO	N-CA-C	7.70	125.23	113.75
2	A	123	GLY	CA-C-N	7.60	127.31	119.56
2	A	123	GLY	C-N-CA	7.60	127.31	119.56
2	A	308	HIS	N-CA-C	7.48	119.43	111.28
1	E	400	DG	O5'-C5'-C4'	-7.46	99.61	110.80
2	A	271	ILE	N-CA-C	7.43	119.18	108.48
2	A	169	PRO	N-CA-C	7.41	119.74	110.70
2	A	134	SER	N-CA-C	-7.23	98.93	110.14
2	B	125	HIS	N-CA-C	-7.01	93.80	107.62
2	B	134	SER	N-CA-C	-6.96	99.35	110.14
2	A	269	ARG	CA-C-N	6.90	126.94	119.90
2	A	269	ARG	C-N-CA	6.90	126.94	119.90
2	B	218	GLU	N-CA-C	6.89	121.73	113.12
2	A	151	LEU	N-CA-C	6.84	120.39	109.24
2	A	161	ILE	N-CA-C	6.78	119.57	108.99
2	B	201	ARG	N-CA-C	6.70	118.66	111.36
2	B	169	PRO	CA-C-O	-6.62	110.96	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	PRO	C-N-CD	6.49	151.59	125.00
2	B	165	VAL	N-CA-C	6.41	119.30	108.86
2	A	156	ALA	CA-C-N	-6.40	112.57	122.87
2	A	156	ALA	C-N-CA	-6.40	112.57	122.87
2	B	295	CYS	CA-CB-SG	-6.22	100.09	114.40
2	B	136	THR	N-CA-C	-6.20	105.29	112.92
2	A	189	ASP	N-CA-C	-6.10	99.33	109.46
2	A	263	VAL	N-CA-C	5.92	117.31	108.54
2	A	168	PRO	N-CA-C	5.92	117.92	110.70
2	B	284	VAL	N-CA-C	5.90	117.28	108.54
2	B	213	HIS	N-CA-C	5.90	119.52	110.20
2	B	247	THR	N-CA-C	5.90	117.21	108.60
2	A	287	ARG	N-CA-C	5.84	118.74	108.75
2	A	157	LYS	N-CA-C	-5.78	100.75	109.95
2	B	261	SER	N-CA-C	5.72	119.87	113.01
2	B	125	HIS	N-CA-CB	5.61	119.95	110.46
2	B	271	ILE	N-CA-C	5.61	116.56	108.48
2	B	220	ASN	N-CA-C	5.58	117.49	108.34
2	B	127	PHE	CA-C-N	-5.54	113.76	122.73
2	B	127	PHE	C-N-CA	-5.54	113.76	122.73
2	B	117	SER	N-CA-C	-5.51	101.30	110.17
2	A	135	SER	N-CA-C	-5.50	102.87	110.35
2	A	136	THR	N-CA-C	-5.46	106.20	112.92
2	B	169	PRO	O-C-N	5.46	127.90	121.46
2	A	292	GLY	N-CA-C	5.42	120.36	110.71
2	A	309	TYR	N-CA-C	5.42	116.87	111.07
1	E	400	DG	O4'-C1'-N9	-5.42	100.27	108.40
2	A	262	CYS	N-CA-C	5.38	118.03	110.23
2	B	169	PRO	CB-CA-C	-5.38	104.36	110.92
2	B	269	ARG	CA-C-O	5.38	124.54	119.59
2	B	287	ARG	CA-C-N	-5.37	113.77	122.36
2	B	287	ARG	C-N-CA	-5.37	113.77	122.36
2	B	186	HIS	CA-CB-CG	-5.37	108.43	113.80
2	B	184	ALA	N-CA-C	5.32	117.77	111.33
2	B	195	PRO	CA-C-O	-5.30	110.89	119.84
2	B	193	ARG	CA-C-N	5.29	127.75	120.39
2	B	193	ARG	C-N-CA	5.29	127.75	120.39
2	A	124	PRO	N-CA-C	-5.25	107.02	113.84
2	A	181	TYR	N-CA-C	5.24	118.04	110.28
2	A	117	SER	N-CA-C	-5.24	103.12	110.50
2	B	194	CYS	CA-C-N	-5.22	113.37	119.32
2	B	194	CYS	C-N-CA	-5.22	113.37	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	203	PHE	N-CA-C	5.13	120.28	112.54
2	A	114	PHE	N-CA-C	5.11	117.63	111.40
2	A	308	HIS	CA-C-N	-5.09	113.83	120.44
2	A	308	HIS	C-N-CA	-5.09	113.83	120.44
2	A	159	CYS	CA-C-N	5.07	126.90	120.51
2	A	159	CYS	C-N-CA	5.07	126.90	120.51
2	A	196	ASN	N-CA-C	5.06	116.80	111.28
2	A	115	ILE	CB-CA-C	-5.05	105.37	111.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	310	ARG	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	E	205	0	113	3	0
1	F	205	0	113	2	0
2	A	1547	0	1519	131	0
2	B	1547	0	1519	142	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	3506	0	3264	270	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 40.

All (270) 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:168:PRO:CB	2:A:169:PRO:HD2	1.62	1.26
2:A:168:PRO:HB3	2:A:169:PRO:HD2	1.17	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:248:GLU:OE1	2:A:249:PHE:HD2	1.36	1.05
2:A:196:ASN:ND2	2:B:195:PRO:HG2	1.72	1.04
2:B:128:GLU:HG3	2:B:164:LYS:HG3	1.38	1.03
2:B:234:GLN:O	2:B:234:GLN:NE2	1.92	1.02
2:B:181:TYR:CE2	2:B:191:VAL:HG22	1.95	1.02
2:A:248:GLU:OE1	2:A:249:PHE:CD2	2.14	1.00
2:A:117:SER:HB3	2:A:287:ARG:HH12	1.30	0.96
2:A:170:PRO:O	2:A:173:THR:HG23	1.66	0.94
2:B:155:ILE:HD11	2:B:259:ASN:HD21	1.33	0.92
2:A:117:SER:O	2:A:287:ARG:NH2	2.03	0.92
2:A:169:PRO:CB	2:A:170:PRO:HA	2.00	0.91
2:A:196:ASN:HD21	2:B:195:PRO:CG	1.85	0.89
2:A:121:TYR:HB3	2:A:287:ARG:HB3	1.55	0.89
2:A:196:ASN:HD21	2:B:195:PRO:HG2	1.34	0.89
2:A:169:PRO:HB3	2:A:170:PRO:HA	1.53	0.89
2:B:132:GLN:H	2:B:162:GLN:HE22	1.17	0.88
2:A:197:HIS:HE1	2:A:262:CYS:SG	1.91	0.88
2:B:150:LYS:HE3	2:B:291:GLU:HB3	1.57	0.87
2:B:213:HIS:NE2	2:B:227:ASP:OD1	2.07	0.86
2:A:148:LEU:O	2:A:148:LEU:HD23	1.76	0.86
2:B:176:ARG:NH2	2:B:235:SER:OG	2.10	0.84
2:A:117:SER:C	2:A:287:ARG:HH22	1.83	0.84
2:B:117:SER:OG	2:B:287:ARG:NH2	2.10	0.84
2:B:181:TYR:CD2	2:B:191:VAL:HG22	2.14	0.83
2:A:279:MET:HG2	2:A:285:LEU:HD11	1.61	0.83
2:B:243:PRO:HB3	2:B:249:PHE:O	1.78	0.83
2:B:155:ILE:HD11	2:B:259:ASN:ND2	1.94	0.82
2:A:168:PRO:CB	2:A:169:PRO:CD	2.52	0.82
2:A:196:ASN:ND2	2:B:195:PRO:CG	2.44	0.80
2:A:148:LEU:O	2:A:148:LEU:CD2	2.30	0.78
2:B:179:PRO:HB2	2:B:271:ILE:HD11	1.64	0.78
2:A:113:GLU:O	2:A:233:ARG:NH2	2.15	0.78
2:A:163:ILE:HD11	2:A:250:THR:HG22	1.65	0.78
2:B:267:ASN:HB2	2:B:269:ARG:NH2	1.98	0.78
2:B:210:PRO:HG2	2:B:213:HIS:CD2	2.21	0.76
2:B:266:MET:O	2:B:269:ARG:HG2	1.85	0.75
2:B:126:HIS:NE2	2:B:166:SER:HB2	2.00	0.75
2:B:272:LEU:HD23	2:B:291:GLU:HB2	1.69	0.73
2:B:132:GLN:OE1	2:B:132:GLN:N	2.21	0.73
2:B:135:SER:HB2	2:B:140:ALA:HB2	1.71	0.73
2:B:192:LYS:HE3	2:B:212:SER:HB2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLN:OE1	2:B:162:GLN:NE2	2.21	0.72
2:B:132:GLN:N	2:B:162:GLN:HE22	1.87	0.72
2:B:128:GLU:HG3	2:B:164:LYS:CG	2.19	0.71
2:A:193:ARG:HH21	2:A:197:HIS:HB3	1.54	0.71
2:B:263:VAL:HA	2:B:267:ASN:OD1	1.92	0.70
2:B:145:SER:HA	2:B:302:ARG:HH22	1.57	0.70
2:B:171:PRO:O	2:B:173:THR:N	2.23	0.70
2:B:247:THR:HG22	2:B:248:GLU:H	1.56	0.70
2:A:193:ARG:NH1	2:A:216:ARG:HH21	1.90	0.70
2:B:207:GLN:N	2:B:207:GLN:OE1	2.24	0.70
2:B:121:TYR:HB3	2:B:287:ARG:CG	2.20	0.70
2:B:272:LEU:HA	2:B:291:GLU:HA	1.72	0.70
2:B:255:ASN:HB3	2:B:257:MET:HE3	1.73	0.69
2:A:191:VAL:O	2:A:234:GLN:NE2	2.25	0.69
2:A:168:PRO:HB2	2:A:169:PRO:HD2	1.73	0.68
2:A:169:PRO:CB	2:A:170:PRO:CA	2.72	0.68
2:B:182:LYS:HG2	2:B:272:LEU:HG	1.76	0.67
2:B:209:ALA:HB3	2:B:216:ARG:HH11	1.59	0.66
2:A:169:PRO:HB3	2:A:170:PRO:CA	2.25	0.66
2:B:144:TYR:O	2:B:302:ARG:NH2	2.28	0.66
2:A:195:PRO:O	2:A:199:LEU:HG	1.96	0.66
2:A:153:CYS:SG	2:A:154:GLN:N	2.70	0.65
2:A:271:ILE:O	2:A:292:GLY:N	2.24	0.65
2:B:121:TYR:HB3	2:B:287:ARG:HG3	1.79	0.65
1:E:400:DG:H2"	1:E:401:DA:C8	2.32	0.65
2:A:196:ASN:HD21	2:B:195:PRO:CD	2.10	0.65
2:B:149:LYS:C	2:B:150:LYS:HD2	2.22	0.64
2:B:193:ARG:HG2	2:B:258:CYS:SG	2.38	0.64
2:B:153:CYS:SG	2:B:154:GLN:N	2.71	0.63
2:B:220:ASN:OD1	2:B:222:LEU:N	2.26	0.63
2:A:216:ARG:HE	2:A:257:MET:HG3	1.62	0.63
2:B:221:ASN:O	2:B:221:ASN:ND2	2.32	0.62
2:B:228:ASP:OD1	2:B:231:THR:N	2.28	0.62
2:B:262:CYS:O	2:B:267:ASN:OD1	2.17	0.61
2:A:247:THR:CG2	2:A:248:GLU:N	2.63	0.60
2:B:130:THR:HG22	2:B:131:PHE:N	2.16	0.60
2:A:125:HIS:CD2	2:A:167:THR:HB	2.35	0.60
2:B:185:GLU:C	2:B:186:HIS:CD2	2.79	0.60
2:A:163:ILE:O	2:A:249:PHE:HB3	2.02	0.59
2:A:209:ALA:HB3	2:A:216:ARG:HH11	1.67	0.59
2:A:231:THR:HG21	2:A:233:ARG:HE	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:145:SER:HB2	2:A:302:ARG:HE	1.67	0.59
2:B:159:CYS:O	2:B:159:CYS:SG	2.61	0.59
2:B:182:LYS:CG	2:B:272:LEU:HG	2.34	0.58
2:A:181:TYR:HD1	2:A:271:ILE:HG22	1.68	0.58
1:F:416:DG:H1'	1:F:417:DT:H5'	1.86	0.57
2:B:130:THR:HG22	2:B:131:PHE:H	1.68	0.57
2:B:117:SER:C	2:B:287:ARG:HH12	2.12	0.57
2:A:172:GLY:HA3	2:A:280:ARG:HH11	1.70	0.57
2:A:138:LYS:HA	2:A:299:GLY:HA3	1.86	0.57
2:B:210:PRO:HG2	2:B:213:HIS:CG	2.39	0.57
2:B:270:PRO:HB2	2:B:291:GLU:OE2	2.05	0.57
2:A:161:ILE:HD13	2:A:254:TYR:HD2	1.70	0.57
2:A:175:ILE:HG12	2:A:277:LEU:HD12	1.86	0.57
2:A:262:CYS:O	2:A:267:ASN:HA	2.05	0.57
2:B:195:PRO:HD2	2:B:264:GLY:HA3	1.87	0.57
2:A:231:THR:HG23	2:A:233:ARG:H	1.71	0.56
2:B:179:PRO:CB	2:B:271:ILE:HD11	2.35	0.56
1:E:405:DG:P	2:B:293:ARG:HH12	2.28	0.56
2:B:192:LYS:HD3	2:B:234:GLN:HG2	1.87	0.56
2:B:198:GLU:OE2	2:B:199:LEU:HG	2.06	0.56
2:A:181:TYR:CD1	2:A:271:ILE:HG22	2.40	0.56
2:B:126:HIS:CE1	2:B:166:SER:H	2.24	0.55
2:A:133:GLN:OE1	2:A:133:GLN:N	2.39	0.55
2:A:260:SER:HA	2:A:266:MET:HE2	1.89	0.55
2:A:160:PRO:HA	2:A:252:ILE:O	2.08	0.55
2:A:163:ILE:CD1	2:A:250:THR:HG22	2.35	0.55
2:B:145:SER:HA	2:B:302:ARG:NH2	2.21	0.55
2:B:300:ARG:HA	2:B:303:LYS:HE2	1.88	0.54
2:A:171:PRO:O	2:A:280:ARG:NH1	2.40	0.54
2:A:193:ARG:NH1	2:A:216:ARG:NH2	2.56	0.54
2:B:182:LYS:HD2	2:B:291:GLU:CD	2.31	0.54
2:A:309:TYR:CD1	2:A:310:ARG:N	2.75	0.54
2:B:228:ASP:OD1	2:B:230:VAL:N	2.41	0.54
2:A:271:ILE:HG13	2:A:292:GLY:O	2.08	0.54
2:B:273:ILE:HD11	2:B:290:PHE:CZ	2.43	0.54
2:A:123:GLY:HA3	2:A:285:LEU:O	2.08	0.54
2:B:288:ARG:HG3	2:B:289:SER:N	2.22	0.54
2:B:148:LEU:HD11	2:B:306:GLU:HG2	1.90	0.54
2:A:241:GLU:OE1	2:A:242:PRO:HD2	2.08	0.54
2:A:126:HIS:HE1	2:A:128:GLU:OE1	1.92	0.53
2:B:162:GLN:OE1	2:B:162:GLN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:THR:CG2	2:B:131:PHE:H	2.22	0.53
2:A:247:THR:CG2	2:A:248:GLU:H	2.22	0.53
1:E:406:DG:C8	1:E:407:DT:H72	2.44	0.53
2:A:209:ALA:HB3	2:A:216:ARG:NH1	2.24	0.53
2:B:150:LYS:HA	2:B:291:GLU:O	2.09	0.53
2:B:180:VAL:O	2:B:271:ILE:HG13	2.09	0.53
2:B:148:LEU:HB3	2:B:150:LYS:HD3	1.90	0.52
2:B:197:HIS:O	2:B:198:GLU:C	2.52	0.52
2:B:179:PRO:CD	2:B:234:GLN:HE22	2.22	0.52
2:B:187:VAL:O	2:B:233:ARG:NH2	2.42	0.52
2:A:170:PRO:O	2:A:173:THR:CG2	2.49	0.52
2:A:247:THR:HG22	2:A:248:GLU:N	2.24	0.52
2:B:213:HIS:CE1	2:B:234:GLN:HB2	2.44	0.52
2:A:160:PRO:HB3	2:A:253:LEU:HD23	1.92	0.52
2:A:186:HIS:CD2	2:A:269:ARG:HH11	2.28	0.52
2:B:128:GLU:CG	2:B:164:LYS:HG3	2.27	0.52
2:A:309:TYR:HE1	2:A:310:ARG:HE	1.58	0.52
2:B:185:GLU:C	2:B:186:HIS:HD2	2.17	0.52
2:B:252:ILE:HD12	2:B:254:TYR:CE2	2.45	0.52
2:A:186:HIS:CG	2:A:269:ARG:HD2	2.45	0.51
2:A:273:ILE:HB	2:A:290:PHE:CE1	2.44	0.51
2:B:213:HIS:HE2	2:B:227:ASP:CG	2.10	0.51
2:A:144:TYR:OH	2:A:149:LYS:HG3	2.10	0.51
2:B:185:GLU:O	2:B:186:HIS:HD2	1.94	0.51
2:B:216:ARG:NE	2:B:257:MET:SD	2.64	0.50
2:A:279:MET:HG2	2:A:285:LEU:CD1	2.37	0.50
2:B:193:ARG:NH2	2:B:197:HIS:HB3	2.27	0.50
2:B:276:THR:HG22	2:B:287:ARG:HB3	1.94	0.50
2:A:131:PHE:HE1	2:A:161:ILE:CG1	2.25	0.50
2:A:169:PRO:HB2	2:A:170:PRO:HA	1.89	0.50
2:A:247:THR:HG23	2:A:248:GLU:H	1.76	0.50
2:A:272:LEU:HA	2:A:291:GLU:HA	1.94	0.50
2:A:196:ASN:HD21	2:B:195:PRO:HD2	1.74	0.50
2:B:155:ILE:H	2:B:155:ILE:HD12	1.76	0.50
2:A:186:HIS:ND1	2:A:269:ARG:HD2	2.27	0.50
2:A:241:GLU:HG3	2:A:242:PRO:O	2.12	0.50
2:A:274:ILE:O	2:A:274:ILE:HG13	2.13	0.49
2:B:176:ARG:O	2:B:275:ILE:HA	2.13	0.49
2:A:144:TYR:OH	2:A:149:LYS:HA	2.13	0.49
2:A:142:TRP:CZ2	2:A:160:PRO:HD2	2.48	0.49
2:B:247:THR:HG22	2:B:248:GLU:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:GLN:HA	2:B:250:THR:O	2.14	0.48
2:A:138:LYS:HE3	2:A:138:LYS:HB3	1.56	0.48
2:B:186:HIS:ND1	2:B:269:ARG:HD3	2.28	0.48
2:A:185:GLU:HG3	2:A:186:HIS:CD2	2.48	0.48
2:A:193:ARG:HH11	2:A:216:ARG:NH2	2.12	0.48
2:A:279:MET:CG	2:A:285:LEU:HD11	2.37	0.48
2:A:197:HIS:HB2	2:A:258:CYS:SG	2.54	0.48
2:A:216:ARG:NE	2:A:257:MET:HG3	2.29	0.47
2:B:117:SER:O	2:B:287:ARG:NH1	2.44	0.47
2:B:186:HIS:CD2	2:B:186:HIS:N	2.79	0.47
2:A:148:LEU:O	2:A:148:LEU:HD22	2.13	0.47
2:B:150:LYS:CE	2:B:291:GLU:HB3	2.36	0.47
2:B:126:HIS:CE1	2:B:166:SER:N	2.82	0.47
2:B:198:GLU:CD	2:B:199:LEU:HG	2.40	0.47
2:B:228:ASP:OD1	2:B:230:VAL:HG22	2.15	0.47
2:A:150:LYS:HG3	2:A:291:GLU:O	2.15	0.46
2:B:156:ALA:HA	2:B:257:MET:CE	2.45	0.46
2:A:135:SER:OG	2:A:140:ALA:HB2	2.15	0.46
2:B:144:TYR:OH	2:B:149:LYS:HA	2.15	0.46
2:B:130:THR:CG2	2:B:131:PHE:N	2.77	0.46
2:A:193:ARG:HG3	2:A:258:CYS:SG	2.56	0.46
2:B:182:LYS:HG2	2:B:272:LEU:CG	2.44	0.46
2:B:198:GLU:HB2	2:B:211:ALA:O	2.16	0.46
2:A:150:LYS:HA	2:A:291:GLU:O	2.15	0.46
2:A:231:THR:HG21	2:A:233:ARG:HH21	1.80	0.46
2:B:186:HIS:HA	2:B:189:ASP:OD2	2.15	0.46
2:B:197:HIS:C	2:B:199:LEU:N	2.69	0.46
2:A:128:GLU:HB3	2:A:164:LYS:HG2	1.98	0.45
2:A:128:GLU:CD	2:A:164:LYS:HE3	2.41	0.45
2:A:178:MET:HB2	2:A:235:SER:HB3	1.98	0.45
2:A:193:ARG:NH2	2:A:197:HIS:O	2.48	0.45
2:A:193:ARG:NH1	2:A:211:ALA:O	2.50	0.45
2:B:131:PHE:N	2:B:131:PHE:CD2	2.85	0.45
2:B:193:ARG:HH21	2:B:197:HIS:HB3	1.81	0.45
2:A:152:TYR:CE1	2:A:293:ARG:HD3	2.52	0.45
2:A:168:PRO:HB3	2:A:169:PRO:CD	2.12	0.45
2:A:138:LYS:NZ	2:A:300:ARG:HB2	2.32	0.45
2:A:197:HIS:CB	2:A:258:CYS:SG	3.05	0.45
2:B:125:HIS:O	2:B:126:HIS:C	2.60	0.44
2:B:167:THR:HA	2:B:168:PRO:HD2	1.68	0.44
2:B:276:THR:HG22	2:B:287:ARG:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:147:LEU:HD23	2:A:147:LEU:C	2.43	0.44
2:A:158:THR:HG23	2:A:253:LEU:HB3	1.99	0.44
1:F:416:DG:OP2	2:A:295:CYS:HB2	2.18	0.44
2:A:113:GLU:O	2:A:233:ARG:CZ	2.65	0.44
2:A:143:THR:OG1	2:A:302:ARG:NH2	2.46	0.44
2:A:200:GLY:O	2:A:204:ASN:ND2	2.51	0.44
2:B:196:ASN:O	2:B:200:GLY:N	2.51	0.43
2:A:231:THR:CG2	2:A:233:ARG:HE	2.31	0.43
2:B:186:HIS:ND1	2:B:269:ARG:CD	2.81	0.43
2:A:131:PHE:HE1	2:A:161:ILE:HG12	1.82	0.43
2:A:142:TRP:CE2	2:A:160:PRO:HD2	2.53	0.43
2:B:159:CYS:SG	2:B:256:PHE:HE2	2.40	0.43
2:B:163:ILE:HD12	2:B:163:ILE:HA	1.65	0.43
2:A:207:GLN:HG3	2:A:209:ALA:HB3	2.00	0.43
2:B:224:GLN:HB2	2:B:237:VAL:HG22	2.00	0.43
2:A:116:PRO:HD3	2:A:233:ARG:HH11	1.84	0.43
2:B:195:PRO:HA	2:B:198:GLU:OE1	2.19	0.43
2:B:178:MET:HE2	2:B:178:MET:HB2	1.97	0.43
2:A:143:THR:HG1	2:A:302:ARG:HH21	1.64	0.42
2:B:300:ARG:HG3	2:B:303:LYS:HE3	2.01	0.42
2:B:262:CYS:O	2:B:267:ASN:HA	2.19	0.42
2:B:178:MET:O	2:B:274:ILE:HG13	2.19	0.42
2:B:179:PRO:CD	2:B:234:GLN:NE2	2.82	0.42
2:B:264:GLY:N	2:B:267:ASN:OD1	2.52	0.42
2:A:131:PHE:CE1	2:A:161:ILE:CG1	3.02	0.42
2:A:145:SER:HB2	2:A:302:ARG:NE	2.33	0.42
2:B:247:THR:CG2	2:B:248:GLU:H	2.28	0.42
2:A:123:GLY:O	2:A:126:HIS:N	2.46	0.42
2:A:125:HIS:HD2	2:A:167:THR:HB	1.82	0.42
2:B:175:ILE:O	2:B:237:VAL:HA	2.20	0.42
2:A:150:LYS:HB2	2:A:291:GLU:HG3	2.02	0.42
2:B:179:PRO:CG	2:B:234:GLN:HE22	2.32	0.42
2:B:150:LYS:HE3	2:B:291:GLU:OE1	2.20	0.41
2:B:121:TYR:HB3	2:B:287:ARG:HG2	2.00	0.41
2:B:193:ARG:NH1	2:B:216:ARG:NH2	2.68	0.41
2:B:273:ILE:HD11	2:B:290:PHE:CE2	2.56	0.41
2:A:181:TYR:OH	2:A:266:MET:HA	2.21	0.41
2:B:269:ARG:HH11	2:B:269:ARG:HD2	1.71	0.41
2:B:288:ARG:HG3	2:B:289:SER:H	1.84	0.41
2:A:158:THR:OG1	2:A:218:GLU:OE1	2.21	0.41
2:A:182:LYS:HB2	2:A:272:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:PRO:C	2:B:173:THR:N	2.78	0.41
2:A:122:PRO:HG3	2:A:288:ARG:NH2	2.36	0.41
2:A:170:PRO:O	2:A:171:PRO:C	2.64	0.41
2:B:207:GLN:HG3	2:B:216:ARG:HD3	2.03	0.41
2:B:259:ASN:O	2:B:262:CYS:HB2	2.21	0.41
2:A:121:TYR:O	2:A:287:ARG:N	2.49	0.41
2:A:128:GLU:HB3	2:A:164:LYS:CG	2.51	0.41
2:A:131:PHE:HE1	2:A:161:ILE:HG13	1.86	0.41
2:A:228:ASP:CB	2:A:231:THR:HG22	2.51	0.41
2:B:171:PRO:C	2:B:173:THR:H	2.29	0.41
2:A:117:SER:HB3	2:A:287:ARG:NH1	2.14	0.40
2:A:130:THR:N	2:A:162:GLN:O	2.49	0.40
2:A:297:CYS:HB2	2:A:300:ARG:HH21	1.86	0.40
2:B:215:ILE:O	2:B:236:VAL:HG21	2.21	0.40
2:B:267:ASN:HB2	2:B:269:ARG:CZ	2.49	0.40
2:B:300:ARG:O	2:B:303:LYS:HG2	2.22	0.40
2:A:152:TYR:HE1	2:A:293:ARG:HD3	1.87	0.40
2:A:288:ARG:HD3	2:A:288:ARG:HA	1.94	0.40
2:B:176:ARG:HD3	2:B:278:GLU:CD	2.46	0.40
2:B:207:GLN:HE21	2:B:216:ARG:NE	2.20	0.40
2:B:218:GLU:HG3	2:B:255:ASN:OD1	2.21	0.40
2:B:115:ILE:HA	2:B:116:PRO:HD3	1.90	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	
2	A	196/210 (93%)	193 (98%)	2 (1%)	1 (0%)	24	60
2	B	196/210 (93%)	189 (96%)	5 (3%)	2 (1%)	12	45
All	All	392/420 (93%)	382 (97%)	7 (2%)	3 (1%)	16	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	169	PRO
2	B	172	GLY
2	B	245	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	
2	A	173/186 (93%)	162 (94%)	11 (6%)	16	40
2	B	173/186 (93%)	155 (90%)	18 (10%)	7	25
All	All	346/372 (93%)	317 (92%)	29 (8%)	10	33

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	129	VAL
2	A	194	CYS
2	A	196	ASN
2	A	221	ASN
2	A	237	VAL
2	A	247	THR
2	A	249	PHE
2	A	262	CYS
2	A	269	ARG
2	A	271	ILE
2	A	274	ILE
2	B	128	GLU
2	B	129	VAL
2	B	134	SER
2	B	158	THR
2	B	165	VAL
2	B	175	ILE
2	B	178	MET
2	B	202	ASP
2	B	218	GLU

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Mol	Chain	Res	Type
2	B	230	VAL
2	B	234	GLN
2	B	237	VAL
2	B	245	VAL
2	B	250	THR
2	B	251	THR
2	B	252	ILE
2	B	262	CYS
2	B	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	125	HIS
2	A	186	HIS
2	A	196	ASN
2	A	267	ASN
2	B	259	ASN

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 oligosaccharides 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](#)

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	E	10/20 (50%)	-0.13	0	100 100	74, 90, 97, 119	0
1	F	10/20 (50%)	0.00	0	100 100	73, 96, 113, 122	0
2	A	198/210 (94%)	0.11	1 (0%)	87 73	27, 108, 209, 272	1 (0%)
2	B	198/210 (94%)	0.27	4 (2%)	65 48	28, 102, 183, 262	1 (0%)
All	All	416/460 (90%)	0.17	5 (1%)	76 59	27, 102, 194, 272	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	4.6
2	B	256	PHE	3.5
2	B	215	ILE	3.1
2	A	136	THR	2.4
2	B	253	LEU	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(Å ²)	Q<0.9
3	ZN	B	401	1/1	0.96	0.14	103,103,103,103	0
3	ZN	A	401	1/1	0.97	0.13	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.