



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:40 PM EDT

PDB ID : 3FRK / pdb_00003frk
Title : X-ray structure of QdtB from *T. thermosaccharolyticum* in complex with a P
LP:TDP-3-aminoquinovose aldimine
Authors : Thoden, J.B.; Holden, H.M.
Deposited on : 2009-01-08
Resolution : 2.15 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

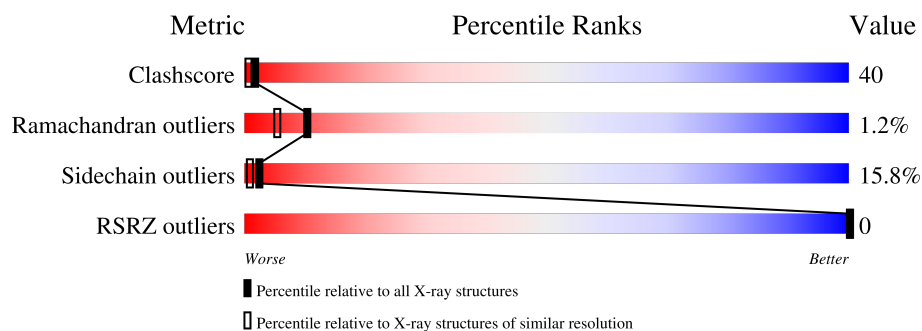
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6157 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.

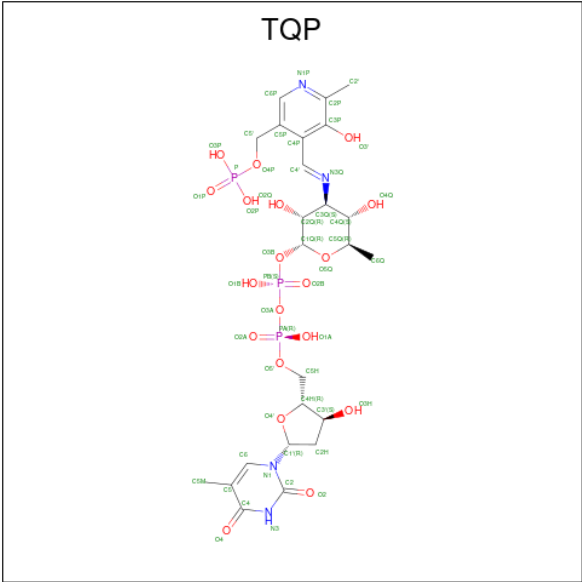
- Molecule 1 is a protein called QdtB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	3	0
			2953	1917	483	545	8			
1	B	364	Total	C	N	O	S	0	1	0
			2924	1895	480	541	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	LEU	-	expression tag	UNP Q6TFC4
A	367	GLU	-	expression tag	UNP Q6TFC4
A	368	HIS	-	expression tag	UNP Q6TFC4
A	369	HIS	-	expression tag	UNP Q6TFC4
A	370	HIS	-	expression tag	UNP Q6TFC4
A	371	HIS	-	expression tag	UNP Q6TFC4
A	372	HIS	-	expression tag	UNP Q6TFC4
A	373	HIS	-	expression tag	UNP Q6TFC4
B	366	LEU	-	expression tag	UNP Q6TFC4
B	367	GLU	-	expression tag	UNP Q6TFC4
B	368	HIS	-	expression tag	UNP Q6TFC4
B	369	HIS	-	expression tag	UNP Q6TFC4
B	370	HIS	-	expression tag	UNP Q6TFC4
B	371	HIS	-	expression tag	UNP Q6TFC4
B	372	HIS	-	expression tag	UNP Q6TFC4
B	373	HIS	-	expression tag	UNP Q6TFC4

- Molecule 2 is (2R,3R,4S,5S,6R)-3,5-dihydroxy-4-[(1E)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene]amino}-6-methyltetrahydro-2H-pyran-2-yl [(2R,3S,5R)-3-hydroxy-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-2-yl]methyl dihydrogen diphosphate (CCD ID: TQP) (formula: C₂₄H₃₅N₄O₁₉P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			50	24	4	19	3		
2	B	1	Total	C	N	O	P	0	0
			50	24	4	19	3		

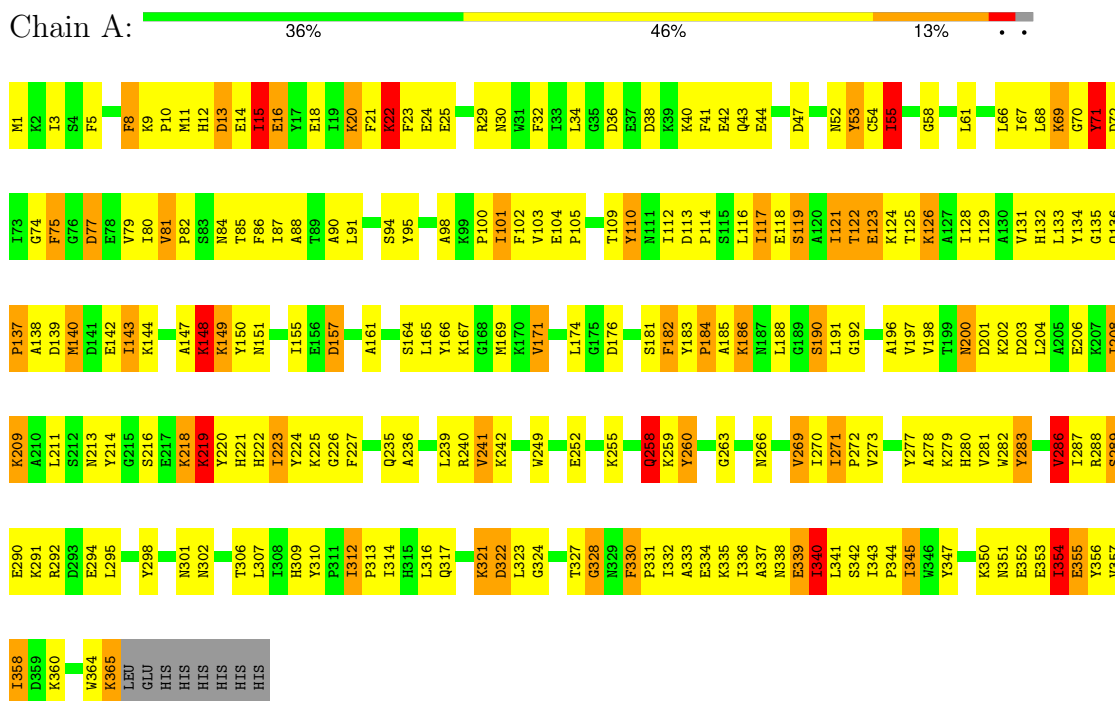
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total	O	0	0
			110	110		
3	B	70	Total	O	0	0
			70	70		

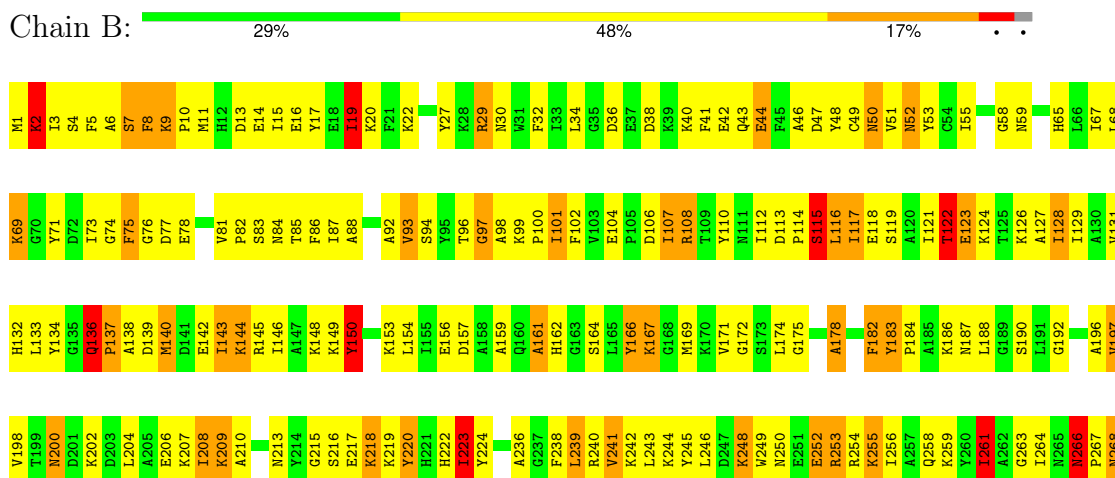
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: QdtB



• Molecule 1: QdtB



I362	A333	E334	K335	L336	A337	K338	E339	L340	L341	S342	I343	E344	K345	L346	A347	K348	M349	E350	E351	L352	E353	L354	E355	L356	V357	L358	D359	K360	L361	N362	A363	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	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	109.10Å 109.10Å 177.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.15 30.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.15) 9.2 (30.00-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.213 , 0.269 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 109.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6157	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: TQP

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	0.84	0/3037	1.83	85/4101 (2.1%)
1	B	0.82	1/2997 (0.0%)	1.80	71/4048 (1.8%)
All	All	0.83	1/6034 (0.0%)	1.82	156/8149 (1.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	VAL	CA-CB	-5.89	1.47	1.54

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ILE	N-CA-C	13.86	124.26	110.82
1	A	340	ILE	N-CA-C	13.60	127.12	109.58
1	B	13	ASP	N-CA-C	-13.15	96.43	111.03
1	B	138	ALA	N-CA-C	-12.03	93.75	110.35
1	B	283	TYR	N-CA-C	-11.91	98.38	111.36
1	B	161	ALA	N-CA-C	10.95	125.95	112.59
1	A	283	TYR	N-CA-C	-10.51	99.83	111.28
1	B	140	MET	N-CA-C	10.08	122.26	111.28
1	B	174	LEU	N-CA-C	9.64	124.37	112.23
1	A	161	ALA	N-CA-C	8.79	124.25	112.30
1	A	25	GLU	N-CA-C	8.76	120.83	111.28
1	A	273	VAL	N-CA-C	8.59	120.14	108.11
1	A	36	ASP	N-CA-C	8.59	120.33	110.97
1	B	144	LYS	N-CA-C	-8.51	101.97	111.07
1	A	15	ILE	CB-CA-C	-8.47	101.10	111.85
1	A	263	GLY	N-CA-C	8.32	123.42	112.77
1	B	340	ILE	N-CA-C	8.29	119.57	110.21
1	B	358	ILE	CB-CA-C	-8.18	101.09	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ILE	CB-CA-C	-7.95	99.19	110.95
1	B	241	VAL	CB-CA-C	-7.91	101.65	112.02
1	A	354	ILE	CB-CA-C	-7.70	102.12	111.97
1	A	157	ASP	N-CA-C	-7.67	92.50	107.62
1	B	263	GLY	N-CA-C	7.66	123.46	113.27
1	B	122	THR	N-CA-C	-7.66	97.77	109.41
1	A	75	PHE	N-CA-C	7.63	121.00	110.24
1	B	150	TYR	N-CA-C	7.60	121.44	112.93
1	B	58	GLY	N-CA-C	7.55	122.44	112.77
1	A	102	PHE	N-CA-C	7.50	122.56	109.96
1	A	241	VAL	CB-CA-C	-7.36	102.55	111.97
1	A	266	ASN	CA-C-N	7.32	127.03	119.56
1	A	266	ASN	C-N-CA	7.32	127.03	119.56
1	B	128	ILE	N-CA-C	-7.30	97.59	108.46
1	A	278	ALA	N-CA-C	7.28	121.89	110.17
1	A	271	ILE	CA-C-N	7.24	127.00	119.76
1	A	271	ILE	C-N-CA	7.24	127.00	119.76
1	A	171	VAL	N-CA-C	-7.22	99.23	109.63
1	A	55	ILE	CB-CA-C	-7.18	100.72	110.42
1	A	200	ASN	N-CA-C	-7.11	104.75	113.50
1	B	276	ASP	N-CA-C	7.05	120.00	111.82
1	B	330	PHE	C-N-CD	-7.04	96.11	125.00
1	B	117	ILE	N-CA-C	7.04	117.15	110.53
1	B	277	TYR	CB-CA-C	-7.01	97.89	110.37
1	A	53	TYR	N-CA-C	6.97	120.86	109.85
1	B	32	PHE	N-CA-C	6.94	122.85	113.97
1	A	216	SER	N-CA-C	6.90	120.18	109.07
1	A	71	TYR	N-CA-C	-6.86	104.91	113.28
1	B	363	ALA	N-CA-C	6.86	120.74	112.38
1	B	115	SER	N-CA-C	-6.85	103.81	111.28
1	A	191	LEU	N-CA-C	-6.82	103.26	112.26
1	A	137	PRO	N-CA-C	6.67	121.41	111.41
1	A	312	ILE	N-CA-C	6.63	118.18	107.71
1	A	333	ALA	N-CA-C	-6.61	104.08	111.28
1	B	136	GLN	CA-C-N	6.54	126.56	119.89
1	B	136	GLN	C-N-CA	6.54	126.56	119.89
1	B	75	PHE	N-CA-C	6.47	119.61	110.23
1	A	129	ILE	CB-CA-C	-6.46	103.13	111.53
1	B	325	PHE	N-CA-C	-6.45	100.66	109.95
1	A	223	ILE	N-CA-C	6.45	121.84	113.07
1	A	219	LYS	N-CA-C	6.44	119.31	110.24
1	B	220	TYR	N-CA-CB	-6.41	106.86	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	MET	N-CA-C	6.40	119.08	111.33
1	B	178	ALA	CA-C-N	6.40	127.00	122.33
1	B	178	ALA	C-N-CA	6.40	127.00	122.33
1	A	22	LYS	N-CA-C	-6.39	104.00	110.97
1	B	273	VAL	N-CA-C	6.39	117.98	108.46
1	A	258[A]	GLN	N-CA-C	-6.38	104.24	111.07
1	A	258[B]	GLN	N-CA-C	-6.38	104.24	111.07
1	B	49	CYS	N-CA-C	-6.36	105.39	113.02
1	A	16[A]	GLU	CA-C-N	-6.34	112.19	120.44
1	A	16[A]	GLU	C-N-CA	-6.34	112.19	120.44
1	A	16[B]	GLU	CA-C-N	-6.34	112.19	120.44
1	A	16[B]	GLU	C-N-CA	-6.34	112.19	120.44
1	B	286	VAL	N-CA-C	6.32	118.12	108.71
1	B	266	ASN	CA-C-N	6.25	127.65	119.84
1	B	266	ASN	C-N-CA	6.25	127.65	119.84
1	B	239	LEU	CA-CB-CG	-6.24	94.44	116.30
1	A	188	LEU	CA-C-N	-6.22	116.77	122.80
1	A	188	LEU	C-N-CA	-6.22	116.77	122.80
1	A	227	PHE	CA-C-N	-6.20	113.17	122.47
1	A	227	PHE	C-N-CA	-6.20	113.17	122.47
1	B	166	TYR	N-CA-C	-6.20	98.17	108.34
1	A	13	ASP	N-CA-C	-6.09	103.80	111.11
1	A	77	ASP	N-CA-C	-6.07	99.82	109.23
1	B	133	LEU	N-CA-C	6.04	119.01	110.50
1	B	137	PRO	N-CA-C	5.98	120.62	111.11
1	B	118	GLU	N-CA-C	5.98	119.40	111.75
1	A	128	ILE	CB-CA-C	-5.95	101.65	110.33
1	A	358	ILE	CB-CA-C	-5.93	104.29	111.88
1	B	204	LEU	CB-CA-C	-5.92	101.56	110.90
1	B	19	ILE	CB-CA-C	-5.90	104.25	111.87
1	B	52	ASN	CB-CA-C	-5.87	99.96	110.70
1	B	208	ILE	N-CA-C	-5.83	104.82	110.42
1	B	167	LYS	N-CA-C	-5.83	103.38	111.30
1	A	269	VAL	CB-CA-C	-5.78	102.98	110.84
1	B	248	LYS	N-CA-C	5.78	117.58	111.28
1	A	176	ASP	N-CA-C	-5.76	106.38	113.41
1	B	197	VAL	CB-CA-C	-5.75	101.96	110.82
1	B	68	LEU	CB-CA-C	-5.73	102.13	110.96
1	A	360	LYS	CA-C-N	-5.73	113.54	120.70
1	A	360	LYS	C-N-CA	-5.73	113.54	120.70
1	A	190	SER	N-CA-C	-5.72	102.45	110.35
1	B	46	ALA	N-CA-C	-5.72	105.04	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	LEU	N-CA-C	-5.70	104.75	110.97
1	B	29	ARG	N-CA-C	-5.69	106.33	113.28
1	A	121	ILE	N-CA-C	5.64	116.86	109.58
1	B	253	ARG	N-CA-C	-5.62	104.37	111.11
1	A	8	PHE	CA-C-O	5.61	125.83	119.27
1	A	70	GLY	N-CA-C	-5.59	106.84	113.99
1	A	138	ALA	N-CA-C	-5.58	103.02	110.55
1	A	58	GLY	N-CA-C	5.56	121.56	114.66
1	A	340	ILE	CA-C-N	-5.56	112.16	121.94
1	A	340	ILE	C-N-CA	-5.56	112.16	121.94
1	B	278	ALA	N-CA-C	5.52	118.57	109.85
1	A	269	VAL	N-CA-C	5.51	116.24	108.36
1	A	281	VAL	CB-CA-C	5.50	118.02	111.20
1	A	222	HIS	N-CA-C	5.50	118.45	107.62
1	A	290	GLU	N-CA-C	5.49	116.95	111.07
1	A	342	SER	N-CA-C	5.49	117.48	108.52
1	B	309	HIS	N-CA-C	5.49	117.54	108.49
1	A	242	LYS	N-CA-C	5.46	117.99	111.71
1	A	286	VAL	N-CA-C	5.40	117.34	108.97
1	A	260	TYR	N-CA-C	-5.39	105.32	111.14
1	A	181	SER	N-CA-C	-5.38	100.93	109.59
1	B	93	VAL	CB-CA-C	-5.36	104.90	112.14
1	B	241	VAL	N-CA-C	-5.35	105.50	110.53
1	B	182	PHE	N-CA-C	-5.34	105.21	112.26
1	A	307	LEU	N-CA-C	-5.33	100.97	109.07
1	B	342	SER	N-CA-C	5.32	117.91	109.24
1	A	182	PHE	N-CA-C	-5.30	105.53	112.41
1	A	185	ALA	N-CA-C	5.29	119.44	113.15
1	A	110	TYR	N-CA-C	-5.25	106.26	113.56
1	B	97	GLY	N-CA-C	-5.24	108.05	115.43
1	B	50	ASN	N-CA-C	5.23	118.42	111.30
1	A	269	VAL	CA-C-N	-5.22	116.35	122.93
1	A	269	VAL	C-N-CA	-5.22	116.35	122.93
1	B	136	GLN	O-C-N	5.22	125.59	121.88
1	A	85	THR	N-CA-C	5.20	117.23	110.53
1	B	266	ASN	CB-CA-C	5.19	116.40	109.65
1	B	361	ILE	N-CA-C	-5.19	104.83	110.23
1	B	84	ASN	N-CA-C	5.18	119.56	112.88
1	B	261	ILE	CG1-CB-CG2	5.18	126.24	110.70
1	B	2	LYS	N-CA-C	5.16	117.14	108.73
1	A	95	TYR	CA-CB-CG	5.14	123.14	113.90
1	B	274	GLU	N-CA-C	5.13	116.63	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	PHE	C-N-CD	-5.09	104.11	125.00
1	B	200	ASN	N-CA-C	-5.09	107.11	113.72
1	B	76	GLY	N-CA-C	-5.08	107.08	114.90
1	A	328	GLY	CA-C-N	-5.08	112.26	121.14
1	A	328	GLY	C-N-CA	-5.08	112.26	121.14
1	A	66	LEU	CA-CB-CG	-5.06	98.59	116.30
1	A	312	ILE	CA-C-N	5.05	125.45	119.99
1	A	312	ILE	C-N-CA	5.05	125.45	119.99
1	B	270	ILE	CB-CA-C	-5.05	104.24	111.31
1	B	183	TYR	N-CA-C	-5.05	103.80	109.60
1	A	271	ILE	O-C-N	5.02	126.82	121.10
1	B	218	LYS	N-CA-C	5.01	116.75	108.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2953	0	2931	191	0
1	B	2924	0	2904	291	0
2	A	50	0	30	3	0
2	B	50	0	30	4	0
3	A	110	0	0	6	0
3	B	70	0	0	3	0
All	All	6157	0	5895	480	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 (480) 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:B:113:ASP:HB3	1:B:116:LEU:HG	1.16	1.14
1:B:122:THR:HG22	1:B:124:LYS:H	1.08	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PRO:HA	1:A:117:ILE:HD12	1.32	1.10
1:A:292:ARG:NH2	1:A:337:ALA:O	1.88	1.06
1:B:114:PRO:HA	1:B:117:ILE:HD12	1.31	1.06
1:B:336:ILE:HG23	1:B:340:ILE:HD13	1.40	1.03
1:B:288:ARG:HG2	1:B:340:ILE:HD12	1.38	1.00
1:A:114:PRO:HA	1:A:117:ILE:CD1	1.92	1.00
1:A:149:LYS:HG2	1:A:150:TYR:CD2	1.99	0.97
1:B:113:ASP:CB	1:B:116:LEU:HG	1.95	0.97
1:B:292:ARG:NH2	1:B:337:ALA:O	1.99	0.96
1:B:320:TYR:O	1:B:323:LEU:HB2	1.65	0.95
1:B:116:LEU:N	1:B:116:LEU:HD23	1.83	0.93
1:B:113:ASP:HB3	1:B:116:LEU:CG	2.00	0.92
1:A:9:LYS:HB3	1:A:10:PRO:HD3	1.53	0.91
1:B:353:GLU:O	1:B:357:VAL:HG23	1.71	0.91
1:B:114:PRO:HA	1:B:117:ILE:CD1	2.00	0.91
1:B:259:LYS:HG2	1:B:354:ILE:HG21	1.50	0.90
1:B:16:GLU:O	1:B:20:LYS:HG3	1.72	0.88
1:B:267:PRO:HG2	1:B:268:ASN:HD21	1.39	0.87
1:B:149:LYS:HG2	1:B:150:TYR:CE2	2.10	0.86
1:B:356:TYR:CE2	1:B:360:LYS:HD2	2.10	0.85
1:A:149:LYS:HG2	1:A:150:TYR:CE2	2.11	0.84
1:B:104:GLU:OE2	1:B:332:ILE:HB	1.76	0.84
1:B:122:THR:HG22	1:B:124:LYS:N	1.92	0.84
1:A:149:LYS:HE2	1:A:150:TYR:CE2	2.13	0.84
1:A:1:MET:HB3	1:A:356:TYR:CE2	2.14	0.83
1:A:204:LEU:O	1:A:208:ILE:HG13	1.77	0.83
1:B:310:TYR:HB3	1:B:311:PRO:HD2	1.60	0.83
1:B:268:ASN:N	1:B:268:ASN:HD22	1.77	0.83
1:B:38:ASP:O	1:B:42:GLU:HG3	1.79	0.82
1:A:1:MET:HE1	1:A:352:GLU:CD	2.05	0.82
1:B:268:ASN:N	1:B:268:ASN:ND2	2.26	0.81
1:B:122:THR:CG2	1:B:124:LYS:H	1.93	0.81
1:A:271:ILE:HB	1:A:272:PRO:HD2	1.62	0.81
1:A:80:ILE:HD13	1:A:117:ILE:HG23	1.61	0.80
1:A:114:PRO:CA	1:A:117:ILE:HD12	2.10	0.80
1:B:16:GLU:HG2	1:B:17:TYR:HD1	1.46	0.80
1:B:93:VAL:CG1	1:B:100:PRO:HD3	2.12	0.79
1:B:104:GLU:HB3	1:B:332:ILE:HD12	1.64	0.79
1:A:77:ASP:OD1	1:A:126:LYS:HG2	1.84	0.78
1:A:74:GLY:O	1:A:77:ASP:HB2	1.84	0.77
1:A:20:LYS:O	1:A:24:GLU:HG3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PRO:O	1:A:101:ILE:HD13	1.85	0.76
1:B:3:ILE:HD12	1:B:353:GLU:HG2	1.65	0.76
1:A:259:LYS:HD3	1:A:354:ILE:HG21	1.66	0.76
1:B:256:ILE:O	1:B:259:LYS:HB3	1.85	0.76
1:A:184:PRO:HD3	1:A:192:GLY:O	1.85	0.75
1:B:250:ASN:O	1:B:254:ARG:HG3	1.86	0.75
1:B:266:ASN:OD1	1:B:268:ASN:ND2	2.20	0.74
1:A:148:LYS:O	1:A:151:ASN:N	2.21	0.74
1:B:52:ASN:HB2	1:B:53:TYR:CD2	2.23	0.73
1:A:220:TYR:CG	1:B:311:PRO:HG3	2.23	0.73
1:B:267:PRO:HG2	1:B:268:ASN:ND2	2.04	0.73
1:B:354:ILE:HG22	1:B:358:ILE:HD11	1.70	0.73
1:B:354:ILE:HG22	1:B:358:ILE:CD1	2.18	0.73
1:B:301:ASN:N	1:B:301:ASN:HD22	1.85	0.72
1:A:271:ILE:HD12	1:A:271:ILE:C	2.14	0.72
1:B:295:LEU:HB2	1:B:364:TRP:CZ2	2.25	0.72
1:A:321:LYS:O	1:A:324:GLY:N	2.19	0.72
1:B:132:HIS:CD2	1:B:171:VAL:HG23	2.25	0.72
1:B:184:PRO:HD3	1:B:192:GLY:O	1.90	0.72
1:B:258:GLN:O	1:B:261:ILE:HG22	1.89	0.71
1:A:236:ALA:O	1:A:240:ARG:HG3	1.90	0.71
1:B:274:GLU:O	1:B:274:GLU:HG2	1.91	0.71
1:B:202:LYS:O	1:B:206:GLU:HG3	1.90	0.71
1:A:354:ILE:O	1:A:358:ILE:HG13	1.90	0.71
1:A:86:PHE:CE2	1:A:88:ALA:HB2	2.26	0.70
1:A:123:GLU:CD	1:A:123:GLU:H	1.99	0.70
1:B:266:ASN:CG	1:B:267:PRO:HD2	2.17	0.69
1:B:268:ASN:HD22	1:B:268:ASN:H	1.39	0.69
1:B:55:ILE:HG23	1:B:209:LYS:HG3	1.73	0.69
1:B:41:PHE:HA	1:B:44:GLU:HG3	1.73	0.68
1:A:202:LYS:O	1:A:206:GLU:HG3	1.93	0.68
1:A:136:GLN:HB3	1:A:280:HIS:CD2	2.29	0.68
1:B:313:PRO:O	1:B:314:ILE:C	2.34	0.68
1:B:11:MET:O	1:B:14:GLU:HB3	1.93	0.68
1:B:314:ILE:O	1:B:317:GLN:HB2	1.94	0.68
1:B:182:PHE:CE2	1:B:196:ALA:HB2	2.30	0.67
1:B:106:ASP:OD1	1:B:108:ARG:HB2	1.94	0.67
1:B:271:ILE:HG23	1:B:272:PRO:HD2	1.76	0.67
1:A:118:GLU:HB2	3:A:415:HOH:O	1.93	0.67
1:B:2:LYS:C	1:B:3:ILE:HD13	2.19	0.67
1:A:113:ASP:HB3	1:A:116:LEU:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HD13	1:B:150:TYR:CG	2.30	0.67
1:A:219:LYS:O	1:A:220:TYR:HB2	1.95	0.66
1:B:219:LYS:O	1:B:220:TYR:HB2	1.93	0.66
1:A:113:ASP:O	1:A:116:LEU:HB2	1.95	0.66
1:B:223:ILE:HG13	1:B:224:TYR:CG	2.30	0.66
1:B:93:VAL:HG11	1:B:100:PRO:HD3	1.77	0.66
1:A:259:LYS:NZ	1:A:355:GLU:OE2	2.24	0.66
1:B:277:TYR:CD2	1:B:277:TYR:C	2.73	0.66
1:A:218:LYS:HG2	1:A:221:HIS:HB2	1.78	0.65
1:B:140:MET:HA	1:B:143:ILE:HG13	1.77	0.65
1:B:116:LEU:HD23	1:B:116:LEU:H	1.62	0.65
1:B:5:PHE:CE2	1:B:307:LEU:HB2	2.32	0.65
1:B:74:GLY:O	1:B:77:ASP:HB2	1.96	0.65
1:B:19:ILE:HG22	1:B:20:LYS:N	2.11	0.65
1:B:295:LEU:HB2	1:B:364:TRP:CH2	2.31	0.65
1:B:116:LEU:N	1:B:116:LEU:CD2	2.58	0.64
1:A:119:SER:OG	3:A:414:HOH:O	2.14	0.64
1:B:264:ILE:HB	1:B:271:ILE:HD11	1.79	0.64
1:B:272:PRO:HD3	1:B:285:PHE:CE2	2.32	0.64
1:B:137:PRO:HD3	1:B:164:SER:OG	1.97	0.64
1:B:288:ARG:CG	1:B:340:ILE:HD12	2.21	0.64
1:B:336:ILE:CG2	1:B:340:ILE:HD13	2.21	0.62
1:A:69:LYS:O	1:A:72:ASP:N	2.29	0.62
1:B:6:ALA:O	1:B:7:SER:HB2	2.00	0.62
1:B:122:THR:CG2	1:B:123:GLU:N	2.63	0.62
1:A:38:ASP:O	1:A:42:GLU:HG3	1.99	0.62
1:B:122:THR:CG2	1:B:124:LYS:HB2	2.30	0.62
1:B:295:LEU:O	1:B:298:TYR:HB3	1.99	0.62
1:B:93:VAL:HG12	1:B:100:PRO:HD3	1.80	0.62
1:B:261:ILE:HD12	1:B:285:PHE:HE1	1.65	0.61
1:B:167:LYS:HG3	1:B:277:TYR:HB2	1.81	0.61
1:B:358:ILE:HG22	1:B:362:ASN:ND2	2.15	0.61
1:B:117:ILE:HD13	1:B:143:ILE:HG23	1.83	0.61
1:B:326:LYS:O	1:B:329:ASN:HB2	2.00	0.61
1:B:197:VAL:HG12	1:B:198:VAL:N	2.16	0.61
1:A:235:GLN:O	1:A:239:LEU:HG	2.01	0.60
1:B:139:ASP:O	1:B:143:ILE:HG13	2.01	0.60
1:B:5:PHE:CD1	1:B:306:THR:HA	2.36	0.60
1:A:87:ILE:HA	1:A:314:ILE:HD11	1.84	0.60
1:A:86:PHE:HD2	1:A:88:ALA:HB3	1.66	0.60
1:A:8:PHE:O	1:A:9:LYS:C	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:TRP:HD1	1:B:347:TYR:CE2	2.19	0.59
1:A:271:ILE:CB	1:A:272:PRO:HD2	2.27	0.59
1:B:261:ILE:CD1	1:B:285:PHE:HE1	2.15	0.59
1:B:252:GLU:HA	1:B:255:LYS:HG3	1.83	0.59
1:A:40:LYS:O	1:A:44:GLU:HG3	2.03	0.59
1:B:341:LEU:HG	1:B:342:SER:N	2.17	0.59
1:B:346:TRP:O	1:B:347:TYR:C	2.44	0.59
1:A:331:PRO:HA	1:A:334:GLU:HB2	1.84	0.59
1:B:149:LYS:HG2	1:B:150:TYR:CD2	2.37	0.58
1:B:148:LYS:O	1:B:149:LYS:C	2.46	0.58
1:A:139:ASP:O	1:A:143:ILE:HG13	2.04	0.58
1:A:113:ASP:HB3	1:A:116:LEU:CD1	2.33	0.58
2:A:374:TQP:O2A	3:A:426:HOH:O	2.16	0.58
1:B:242:LYS:O	1:B:243:LEU:C	2.47	0.58
1:A:183:TYR:HB3	1:A:186:LYS:HE3	1.85	0.57
1:B:53:TYR:HE2	1:B:200:ASN:O	1.87	0.57
1:A:75:PHE:HZ	1:B:75:PHE:CZ	2.22	0.57
1:A:298:TYR:O	1:A:302:ASN:ND2	2.37	0.57
1:B:115:SER:HB2	1:B:116:LEU:HD23	1.85	0.57
1:B:266:ASN:OD1	1:B:269:VAL:HG23	2.04	0.57
1:A:86:PHE:CD2	1:A:88:ALA:CB	2.87	0.57
1:B:87:ILE:HA	1:B:314:ILE:HD11	1.87	0.57
1:A:335:LYS:O	1:A:338:ASN:HB2	2.03	0.57
1:B:164:SER:HA	1:B:281:VAL:HG13	1.85	0.57
1:A:12:HIS:ND1	1:B:30:ASN:OD1	2.26	0.57
1:A:147:ALA:O	1:A:151:ASN:N	2.36	0.57
1:B:3:ILE:CD1	1:B:353:GLU:HG2	2.34	0.57
1:B:161:ALA:O	1:B:171:VAL:HG11	2.05	0.57
1:B:15:ILE:O	1:B:16:GLU:C	2.45	0.56
1:B:139:ASP:HA	1:B:166:TYR:HE1	1.69	0.56
1:A:105:PRO:HA	1:A:112:ILE:HA	1.86	0.56
1:B:122:THR:HG21	1:B:124:LYS:HB2	1.87	0.56
1:B:104:GLU:CD	1:B:332:ILE:HB	2.30	0.56
1:B:261:ILE:HD12	1:B:285:PHE:CE1	2.41	0.56
1:B:356:TYR:CZ	1:B:360:LYS:HD2	2.40	0.56
1:A:86:PHE:CD2	1:A:88:ALA:HB3	2.40	0.56
1:B:245:TYR:HA	3:B:397:HOH:O	2.04	0.56
1:B:249:TRP:CD1	1:B:347:TYR:CE2	2.93	0.56
1:B:255:LYS:O	1:B:256:ILE:C	2.49	0.56
1:B:142:GLU:O	1:B:146:ILE:HG13	2.05	0.56
1:A:44:GLU:O	1:A:47:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:HE2	1:A:150:TYR:CZ	2.41	0.55
1:A:330:PHE:N	1:A:331:PRO:HD3	2.21	0.55
1:B:334:GLU:O	1:B:338:ASN:ND2	2.38	0.55
1:B:114:PRO:CA	1:B:117:ILE:HD12	2.22	0.55
1:B:272:PRO:CD	1:B:285:PHE:CE2	2.90	0.55
1:A:71:TYR:O	1:A:72:ASP:HB2	2.07	0.55
1:B:166:TYR:CZ	1:B:167:LYS:HE3	2.41	0.55
1:A:86:PHE:HE2	1:A:88:ALA:HB2	1.72	0.55
1:A:43:GLN:O	1:A:43:GLN:NE2	2.38	0.54
1:B:272:PRO:CD	1:B:285:PHE:CZ	2.89	0.54
1:A:149:LYS:HE2	1:A:150:TYR:HE2	1.69	0.54
1:A:252:GLU:HG2	1:A:347:TYR:CD2	2.43	0.54
1:B:77:ASP:OD1	1:B:126:LYS:NZ	2.34	0.54
1:B:142:GLU:O	1:B:145:ARG:HB2	2.07	0.54
1:A:90:ALA:O	1:A:91:LEU:C	2.50	0.54
1:B:331:PRO:N	1:B:334:GLU:OE2	2.39	0.54
1:A:351:ASN:HA	1:A:354:ILE:HG13	1.89	0.54
1:B:71:TYR:CB	1:B:73:ILE:HD12	2.38	0.54
1:B:354:ILE:O	1:B:358:ILE:HD12	2.08	0.54
1:A:353:GLU:O	1:A:356:TYR:HB3	2.07	0.54
1:A:1:MET:HE1	1:A:352:GLU:CG	2.38	0.53
1:A:9:LYS:HG3	1:A:13:ASP:OD2	2.07	0.53
1:A:109:THR:O	1:A:110:TYR:HB2	2.07	0.53
1:B:182:PHE:HE2	1:B:196:ALA:HB2	1.69	0.53
1:A:166:TYR:CZ	1:A:167:LYS:HD2	2.43	0.53
2:A:374:TQP:O2B	2:A:374:TQP:O5'	2.25	0.53
1:A:182:PHE:HE2	1:A:196:ALA:HB2	1.74	0.53
1:B:9:LYS:HB3	1:B:10:PRO:HD3	1.90	0.53
1:B:113:ASP:CG	1:B:116:LEU:HD21	2.34	0.53
1:B:122:THR:HG23	1:B:123:GLU:N	2.23	0.53
1:B:272:PRO:HG3	1:B:285:PHE:CE2	2.43	0.53
1:B:357:VAL:O	1:B:361:ILE:HG12	2.08	0.53
1:A:82:PRO:HA	1:A:103:VAL:O	2.09	0.53
1:A:306:THR:HB	1:A:341:LEU:HD11	1.90	0.53
1:B:8:PHE:CD1	1:B:8:PHE:N	2.76	0.53
1:A:23:PHE:O	1:A:24:GLU:C	2.50	0.53
1:B:65:HIS:HD2	1:B:96:THR:HG22	1.74	0.53
1:B:113:ASP:HB3	1:B:116:LEU:CD1	2.38	0.53
1:B:223:ILE:HG13	1:B:224:TYR:CD1	2.44	0.53
1:B:357:VAL:O	1:B:361:ILE:CG1	2.56	0.53
1:B:107:ILE:HD11	1:B:288:ARG:NE	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:HG13	1:B:107:ILE:O	2.09	0.52
1:B:161:ALA:O	1:B:162:HIS:C	2.51	0.52
1:B:197:VAL:CG1	1:B:198:VAL:N	2.72	0.52
1:B:236:ALA:O	1:B:240:ARG:HG3	2.09	0.52
2:B:374:TQP:N3Q	2:B:374:TQP:O3'	2.39	0.52
1:A:249:TRP:HD1	1:A:347:TYR:CE2	2.27	0.52
1:A:272:PRO:HD3	1:A:286:VAL:O	2.08	0.52
1:B:328:GLY:H	1:B:334:GLU:CD	2.17	0.52
1:B:360:LYS:O	1:B:361:ILE:C	2.50	0.52
1:A:22:LYS:HE2	1:A:22:LYS:HA	1.91	0.52
1:A:223:ILE:HG13	1:A:224:TYR:CE2	2.45	0.52
1:B:223:ILE:CG1	1:B:224:TYR:N	2.72	0.52
1:A:75:PHE:CZ	1:B:75:PHE:CZ	2.98	0.52
1:B:171:VAL:HG13	3:B:403:HOH:O	2.08	0.52
1:A:41:PHE:CE1	1:A:239:LEU:HB3	2.45	0.52
1:A:121:ILE:HG22	1:A:122:THR:N	2.24	0.52
1:A:166:TYR:CE2	1:A:167:LYS:HD2	2.43	0.52
1:A:328:GLY:H	1:A:334:GLU:CD	2.18	0.52
1:A:5:PHE:HA	1:A:344:PRO:HG3	1.91	0.52
1:A:103:VAL:HG11	1:A:117:ILE:HG13	1.92	0.51
1:A:213:ASN:O	1:A:214:TYR:HB2	2.10	0.51
1:A:269:VAL:HG13	1:A:287:ILE:HB	1.93	0.51
1:B:190:SER:HB3	1:B:239:LEU:HD11	1.93	0.51
1:B:310:TYR:CB	1:B:311:PRO:HD2	2.37	0.51
1:A:289:SER:O	1:A:339:GLU:HB3	2.09	0.51
1:B:100:PRO:O	1:B:101:ILE:HD13	2.11	0.51
1:B:136:GLN:HE22	1:B:274:GLU:HA	1.76	0.51
1:A:104:GLU:CD	1:A:332:ILE:HB	2.35	0.51
1:A:21:PHE:HD2	3:A:402:HOH:O	1.93	0.50
1:B:132:HIS:CD2	1:B:171:VAL:CG2	2.93	0.50
1:B:308:ILE:HG12	1:B:341:LEU:HD12	1.92	0.50
1:A:69:LYS:C	1:A:72:ASP:H	2.16	0.50
1:B:52:ASN:CB	1:B:53:TYR:CD2	2.93	0.50
1:B:166:TYR:O	1:B:167:LYS:C	2.54	0.50
1:B:252:GLU:O	1:B:253:ARG:C	2.54	0.50
1:A:103:VAL:HB	1:A:112:ILE:HD11	1.93	0.50
1:B:144:LYS:O	1:B:148:LYS:HG3	2.12	0.50
1:B:285:PHE:C	1:B:285:PHE:CD2	2.90	0.50
1:B:301:ASN:N	1:B:301:ASN:ND2	2.51	0.50
1:A:9:LYS:HB3	1:A:10:PRO:CD	2.32	0.50
1:A:317:GLN:NE2	1:B:222:HIS:HD2	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LYS:O	1:B:44:GLU:CG	2.59	0.50
1:A:55:ILE:N	1:A:55:ILE:HD12	2.26	0.50
1:A:22:LYS:HA	1:A:22:LYS:CE	2.42	0.50
1:A:331:PRO:CA	1:A:334:GLU:HB2	2.42	0.50
1:B:52:ASN:CB	1:B:53:TYR:CE2	2.95	0.50
1:B:139:ASP:O	1:B:143:ILE:CG1	2.60	0.50
1:B:52:ASN:HB2	1:B:53:TYR:CE2	2.47	0.49
1:B:277:TYR:C	1:B:277:TYR:HD2	2.17	0.49
1:A:211:LEU:CD2	1:A:226:GLY:HA2	2.42	0.49
1:A:249:TRP:CD1	1:A:347:TYR:CE2	3.01	0.49
1:B:78:GLU:OE1	1:B:122:THR:HB	2.12	0.49
1:B:71:TYR:CZ	1:B:153:LYS:HD2	2.47	0.49
1:A:270:ILE:HD13	1:A:288:ARG:CZ	2.42	0.49
1:B:113:ASP:OD2	1:B:116:LEU:HD21	2.13	0.49
1:B:323:LEU:N	1:B:323:LEU:HD23	2.18	0.49
1:B:71:TYR:HB3	1:B:73:ILE:HD12	1.94	0.49
1:B:81:VAL:HG12	1:B:129:ILE:HB	1.94	0.49
1:B:29:ARG:O	1:B:30:ASN:C	2.54	0.49
1:A:350:LYS:HB2	1:A:353:GLU:HG3	1.94	0.49
1:B:2:LYS:O	1:B:3:ILE:HD13	2.13	0.49
1:A:295:LEU:HD13	1:A:364:TRP:CD2	2.48	0.48
1:B:139:ASP:OD1	1:B:166:TYR:OH	2.26	0.48
1:A:220:TYR:CD2	1:B:311:PRO:HG3	2.48	0.48
1:A:271:ILE:HB	1:A:272:PRO:CD	2.40	0.48
1:B:354:ILE:HG22	1:B:358:ILE:HD12	1.93	0.48
1:B:298:TYR:CD2	1:B:299:LEU:N	2.82	0.48
1:B:93:VAL:HG11	1:B:100:PRO:CD	2.44	0.48
1:B:115:SER:CB	1:B:116:LEU:HD23	2.43	0.48
1:A:271:ILE:CB	1:A:272:PRO:CD	2.91	0.48
1:B:75:PHE:HA	1:B:97:GLY:O	2.14	0.48
1:B:272:PRO:CG	1:B:285:PHE:CE2	2.97	0.48
1:B:36[B]:ASP:OD2	1:B:40:LYS:HE3	2.13	0.48
1:B:83:SER:OG	1:B:104:GLU:HA	2.12	0.48
2:B:374:TQP:O4Q	2:B:374:TQP:H4'	2.14	0.48
1:B:48:TYR:CZ	1:B:246:LEU:HD23	2.48	0.48
1:B:106:ASP:O	1:B:110:TYR:N	2.47	0.48
1:B:40:LYS:O	1:B:44:GLU:HG2	2.14	0.47
1:B:85:THR:HG23	1:B:86:PHE:O	2.13	0.47
1:A:201:ASP:C	1:A:201:ASP:OD1	2.58	0.47
1:B:159:ALA:O	1:B:186:LYS:HE3	2.14	0.47
1:B:249:TRP:CD1	1:B:347:TYR:CZ	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:VAL:HB	1:B:200:ASN:OD1	2.14	0.47
1:B:127:ALA:HB2	1:B:153:LYS:HB2	1.96	0.47
1:B:272:PRO:CG	1:B:285:PHE:CZ	2.97	0.47
1:A:139:ASP:O	1:A:143:ILE:CG1	2.63	0.47
1:B:283:TYR:CD2	1:B:284:THR:OG1	2.67	0.47
1:A:52:ASN:HB2	1:A:200:ASN:HA	1.97	0.47
1:A:87:ILE:HA	1:A:314:ILE:CD1	2.45	0.47
1:A:113:ASP:HB3	1:A:116:LEU:CG	2.44	0.47
1:A:183:TYR:CZ	2:A:374:TQP:H6QB	2.50	0.47
1:B:51:VAL:HG21	1:B:198:VAL:HB	1.96	0.47
1:B:172:GLY:HA2	1:B:178:ALA:CB	2.45	0.47
1:B:353:GLU:O	1:B:354:ILE:C	2.58	0.47
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.56	0.47
1:A:211:LEU:HD22	1:A:226:GLY:HA2	1.96	0.47
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.52	0.47
1:B:218:LYS:O	1:B:219:LYS:C	2.57	0.47
1:B:323:LEU:HD13	1:B:325:PHE:HE2	1.80	0.47
1:B:144:LYS:O	1:B:145:ARG:C	2.58	0.47
1:B:69:LYS:HD2	1:B:69:LYS:HA	1.81	0.46
1:B:142:GLU:O	1:B:145:ARG:CB	2.63	0.46
1:A:131:VAL:HG22	1:A:157:ASP:HB3	1.95	0.46
1:A:271:ILE:HD12	1:A:271:ILE:O	2.15	0.46
1:B:238:PHE:O	1:B:241:VAL:HB	2.15	0.46
1:B:309:HIS:HA	1:B:310:TYR:CG	2.50	0.46
1:A:69:LYS:HA	1:A:69:LYS:HD2	1.45	0.46
1:A:104:GLU:OE1	1:A:331:PRO:HD2	2.15	0.46
1:B:92:ALA:O	1:B:96:THR:HG23	2.15	0.46
2:B:374:TQP:O2B	2:B:374:TQP:H5H	2.15	0.46
1:A:165:LEU:HA	1:A:169:MET:O	2.15	0.46
1:B:52:ASN:N	1:B:200:ASN:OD1	2.47	0.46
1:B:100:PRO:C	1:B:101:ILE:HD13	2.39	0.46
1:B:261:ILE:CD1	1:B:285:PHE:CE1	2.97	0.46
1:A:133:LEU:C	1:A:135:GLY:H	2.24	0.46
1:A:309:HIS:HA	1:A:310:TYR:CD2	2.51	0.46
1:A:30:ASN:HA	1:A:32:PHE:CE2	2.51	0.46
1:B:5:PHE:CZ	1:B:307:LEU:HB2	2.51	0.46
1:B:52:ASN:HB2	1:B:200:ASN:HA	1.98	0.46
1:A:134:TYR:O	1:A:283:TYR:N	2.49	0.46
1:A:312:ILE:HA	1:A:313:PRO:HD3	1.54	0.46
1:A:331:PRO:C	1:A:334:GLU:HB2	2.42	0.46
1:B:317:GLN:OE1	1:B:317:GLN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASN:CG	1:A:105:PRO:HG3	2.41	0.45
1:A:331:PRO:O	1:A:334:GLU:HB2	2.16	0.45
1:B:113:ASP:CG	1:B:116:LEU:HG	2.39	0.45
1:A:249:TRP:CD1	1:A:347:TYR:CZ	3.05	0.45
1:A:86:PHE:CE2	1:A:88:ALA:CB	2.98	0.45
1:B:74:GLY:O	1:B:98:ALA:HA	2.16	0.45
1:B:332:ILE:O	1:B:336:ILE:HG13	2.16	0.45
1:B:1:MET:HE2	1:B:353:GLU:HG3	1.97	0.45
1:B:213:ASN:ND2	1:B:216:SER:HB3	2.32	0.45
1:A:330:PHE:N	1:A:331:PRO:CD	2.75	0.45
1:B:40:LYS:CD	1:B:240:ARG:NH2	2.79	0.45
1:B:266:ASN:OD1	1:B:267:PRO:HD2	2.16	0.45
1:A:140:MET:HA	1:A:143:ILE:HG13	1.98	0.45
1:A:164:SER:HB3	1:A:171:VAL:HG21	1.99	0.45
1:B:309:HIS:HA	1:B:310:TYR:CD2	2.51	0.45
1:A:3:ILE:HD12	1:A:353:GLU:HB3	1.99	0.45
1:B:40:LYS:HB3	1:B:240:ARG:NH2	2.32	0.45
1:B:71:TYR:HB2	1:B:73:ILE:HD12	1.98	0.45
1:B:99:LYS:HA	1:B:100:PRO:HD2	1.65	0.45
1:A:294:GLU:O	1:A:295:LEU:C	2.58	0.45
1:B:9:LYS:O	1:B:10:PRO:C	2.60	0.45
1:B:75:PHE:CZ	1:B:97:GLY:HA3	2.52	0.45
1:B:361:ILE:O	1:B:362:ASN:C	2.57	0.45
1:A:10:PRO:O	1:A:14:GLU:HB2	2.16	0.44
1:B:123:GLU:H	1:B:123:GLU:HG3	1.26	0.44
1:B:223:ILE:HG12	1:B:224:TYR:N	2.31	0.44
1:B:354:ILE:CG2	1:B:358:ILE:HD11	2.42	0.44
1:B:307:LEU:HD12	2:B:374:TQP:O2B	2.16	0.44
1:B:313:PRO:HD2	1:B:316:LEU:HB2	1.98	0.44
1:B:82:PRO:HG3	1:B:112:ILE:HB	1.99	0.44
1:A:114:PRO:C	1:A:117:ILE:HD12	2.41	0.44
1:B:16:GLU:HG2	1:B:17:TYR:N	2.31	0.44
1:B:182:PHE:O	1:B:183:TYR:C	2.60	0.44
1:A:16[B]:GLU:HG3	1:B:27:TYR:HE2	1.82	0.44
1:A:137:PRO:HD3	1:A:164:SER:OG	2.17	0.44
1:A:350:LYS:O	1:A:351:ASN:C	2.59	0.44
1:B:8:PHE:N	1:B:8:PHE:HD1	2.15	0.44
1:B:298:TYR:CD2	1:B:298:TYR:C	2.95	0.44
1:A:121:ILE:CG2	1:A:122:THR:N	2.80	0.44
1:B:188:LEU:HD11	1:B:242:LYS:CB	2.48	0.44
1:A:80:ILE:CD1	1:A:117:ILE:HG23	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ILE:O	1:B:22:LYS:HB3	2.18	0.44
1:B:207:LYS:O	1:B:208:ILE:C	2.60	0.44
1:B:314:ILE:HG22	1:B:315:HIS:N	2.24	0.44
1:B:77:ASP:OD1	1:B:126:LYS:HG3	2.17	0.44
1:A:112:ILE:O	1:A:112:ILE:HG23	2.18	0.44
1:A:271:ILE:HD13	3:A:404:HOH:O	2.18	0.44
1:B:313:PRO:O	1:B:316:LEU:N	2.50	0.44
1:A:113:ASP:C	1:A:113:ASP:OD1	2.61	0.43
1:B:113:ASP:CG	1:B:116:LEU:CD2	2.91	0.43
1:B:223:ILE:HD11	1:B:224:TYR:CE2	2.53	0.43
1:B:252:GLU:O	1:B:256:ILE:HG13	2.18	0.43
1:B:266:ASN:HA	1:B:267:PRO:HD3	1.81	0.43
1:B:4:SER:HB2	1:B:6:ALA:O	2.18	0.43
1:B:239:LEU:HD23	1:B:239:LEU:HA	1.67	0.43
1:B:8:PHE:O	1:B:9:LYS:C	2.61	0.43
1:A:282:TRP:O	1:A:283:TYR:C	2.59	0.43
1:B:10:PRO:O	1:B:14:GLU:HB2	2.18	0.43
1:A:148:LYS:O	1:A:149:LYS:C	2.61	0.43
1:A:208:ILE:O	1:A:209:LYS:C	2.61	0.43
1:B:210:ALA:O	1:B:215:GLY:CA	2.66	0.43
1:B:210:ALA:O	1:B:215:GLY:N	2.52	0.43
1:B:358:ILE:CG2	1:B:362:ASN:ND2	2.81	0.43
1:B:106:ASP:O	1:B:107:ILE:C	2.61	0.43
1:B:139:ASP:HA	1:B:166:TYR:CE1	2.53	0.43
1:B:270:ILE:HD13	1:B:288:ARG:NH2	2.34	0.43
1:A:67:ILE:HG21	1:A:155:ILE:HD13	2.00	0.43
1:A:79:VAL:O	1:A:100:PRO:HA	2.18	0.43
1:A:104:GLU:OE1	1:A:332:ILE:HD12	2.19	0.43
1:B:102:PHE:HE1	1:B:323:LEU:HD12	1.83	0.43
1:B:286:VAL:O	1:B:286:VAL:HG23	2.18	0.43
1:B:122:THR:HG22	1:B:124:LYS:HB2	2.01	0.43
1:A:80:ILE:C	1:A:81:VAL:CG1	2.92	0.43
1:B:40:LYS:O	1:B:44:GLU:HG3	2.19	0.43
1:A:148:LYS:O	1:A:150:TYR:N	2.51	0.42
1:A:259:LYS:HE2	1:A:351:ASN:OD1	2.19	0.42
1:B:250:ASN:O	1:B:253:ARG:HB2	2.19	0.42
1:A:197:VAL:HG12	1:A:198:VAL:N	2.33	0.42
1:A:260:TYR:CZ	1:A:343:ILE:HD12	2.54	0.42
1:A:291:LYS:HA	1:A:291:LYS:HD2	1.90	0.42
1:B:43:GLN:HG2	1:B:44:GLU:N	2.34	0.42
1:B:292:ARG:HB2	1:B:339:GLU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:GLN:HB2	3:B:401:HOH:O	2.19	0.42
1:A:69:LYS:C	1:A:71:TYR:N	2.72	0.42
1:A:353:GLU:O	1:A:357:VAL:HG23	2.19	0.42
1:A:365:LYS:HE2	1:A:365:LYS:HB3	1.38	0.42
1:A:114:PRO:O	1:A:117:ILE:HD12	2.20	0.42
1:B:41:PHE:CA	1:B:44:GLU:HG3	2.46	0.42
1:A:67:ILE:CG2	1:A:155:ILE:HD13	2.49	0.42
1:A:277:TYR:C	1:A:277:TYR:CD2	2.97	0.42
1:A:321:LYS:HD3	3:A:431:HOH:O	2.18	0.42
1:B:139:ASP:OD1	1:B:139:ASP:C	2.61	0.42
1:B:187:ASN:HD21	1:B:253:ARG:HD2	1.85	0.42
1:B:294:GLU:H	1:B:294:GLU:HG2	1.53	0.42
1:B:316:LEU:HA	1:B:316:LEU:HD23	1.58	0.42
1:B:346:TRP:O	1:B:349:MET:HG3	2.19	0.42
1:B:113:ASP:HA	1:B:114:PRO:HD3	1.84	0.42
1:A:29:ARG:O	1:A:30:ASN:C	2.63	0.42
1:A:336:ILE:O	1:A:340:ILE:HB	2.20	0.42
1:B:140:MET:HE2	1:B:156:GLU:HG2	2.02	0.42
1:A:23:PHE:CD1	1:A:23:PHE:C	2.97	0.42
1:A:321:LYS:O	1:A:322:ASP:C	2.62	0.42
1:B:134:TYR:CD1	1:B:284:THR:HB	2.55	0.42
1:B:150:TYR:CD2	1:B:150:TYR:N	2.88	0.42
1:A:166:TYR:CE2	1:A:167:LYS:CD	3.03	0.41
1:B:4:SER:O	1:B:5:PHE:C	2.62	0.41
1:B:86:PHE:CE2	1:B:88:ALA:HB2	2.55	0.41
1:B:131:VAL:HG22	1:B:157:ASP:HB3	2.01	0.41
1:B:326:LYS:O	1:B:327:THR:C	2.60	0.41
1:A:139:ASP:CG	1:A:142:GLU:HG3	2.46	0.41
1:B:358:ILE:HG22	1:B:358:ILE:O	2.18	0.41
1:A:350:LYS:C	1:A:354:ILE:HG13	2.46	0.41
1:B:300:ASN:C	1:B:302:ASN:N	2.77	0.41
1:A:100:PRO:C	1:A:101:ILE:HD13	2.43	0.41
1:B:154:LEU:HG	1:B:175:GLY:HA3	2.02	0.41
1:A:91:LEU:O	1:A:94:SER:N	2.54	0.41
1:A:301:ASN:HD22	1:A:301:ASN:HA	1.59	0.41
1:B:153:LYS:HA	1:B:153:LYS:HD3	1.61	0.41
1:B:286:VAL:O	1:B:286:VAL:CG2	2.68	0.41
1:B:331:PRO:HA	1:B:334:GLU:OE2	2.21	0.41
1:B:67:ILE:HA	1:B:208:ILE:HD11	2.02	0.41
1:B:306:THR:HB	1:B:342:SER:O	2.21	0.41
1:A:68:LEU:HD23	1:A:68:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:PHE:O	1:A:331:PRO:C	2.63	0.41
1:B:107:ILE:HG13	1:B:288:ARG:NH1	2.36	0.41
1:A:53:TYR:OH	1:A:202:LYS:HB2	2.20	0.41
1:A:125:THR:HG22	1:A:126:LYS:N	2.35	0.41
1:B:34:LEU:HA	1:B:34:LEU:HD23	1.77	0.41
1:B:172:GLY:HA2	1:B:178:ALA:HB2	2.02	0.41
1:B:182:PHE:CZ	1:B:196:ALA:HB2	2.55	0.41
1:B:352:GLU:O	1:B:353:GLU:C	2.63	0.41
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.57	0.41
1:B:188:LEU:HD11	1:B:242:LYS:HB3	2.02	0.41
1:A:132:HIS:CD2	1:A:171:VAL:HG13	2.56	0.40
1:A:142:GLU:H	1:A:142:GLU:HG2	1.44	0.40
1:A:190:SER:OG	1:A:192:GLY:N	2.49	0.40
1:B:166:TYR:O	1:B:169:MET:N	2.41	0.40
1:B:323:LEU:HD22	1:B:323:LEU:HA	1.38	0.40
1:A:54:CYS:HA	1:A:197:VAL:O	2.22	0.40
1:A:149:LYS:CE	1:A:150:TYR:CE2	2.94	0.40
1:A:182:PHE:CE2	1:A:196:ALA:HB2	2.54	0.40
1:A:323:LEU:HA	1:A:323:LEU:HD23	1.57	0.40
1:A:18:GLU:CD	1:A:241:VAL:HG13	2.47	0.40
1:A:105:PRO:HA	1:A:112:ILE:CA	2.50	0.40
1:B:292:ARG:HH22	1:B:338:ASN:HA	1.87	0.40
1:B:312:ILE:HA	1:B:313:PRO:HD3	1.65	0.40
1:B:40:LYS:O	1:B:41:PHE:C	2.63	0.40
1:A:203:ASP:O	1:A:204:LEU:C	2.64	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
1	A	366/373 (98%)	326 (89%)	36 (10%)	4 (1%)	11 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	363/373 (97%)	320 (88%)	38 (10%)	5 (1%)	9	4
All	All	729/746 (98%)	646 (89%)	74 (10%)	9 (1%)	10	5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	ILE
1	B	345	ILE
1	A	149	LYS
1	B	7	SER
1	B	275	ALA
1	A	98	ALA
1	A	148	LYS
1	B	331	PRO
1	B	9	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/316 (98%)	270 (87%)	40 (13%)	4	1
1	B	306/316 (97%)	248 (81%)	58 (19%)	1	0
All	All	616/632 (98%)	518 (84%)	98 (16%)	2	1

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	MET
1	A	15	ILE
1	A	20	LYS
1	A	22	LYS
1	A	55	ILE
1	A	69	LYS
1	A	71	TYR

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Mol	Chain	Res	Type
1	A	81	VAL
1	A	101	ILE
1	A	119	SER
1	A	122	THR
1	A	123	GLU
1	A	124	LYS
1	A	126	LYS
1	A	143	ILE
1	A	144	LYS
1	A	148	LYS
1	A	174	LEU
1	A	184	PRO
1	A	186	LYS
1	A	208	ILE
1	A	209	LYS
1	A	218	LYS
1	A	219	LYS
1	A	225	LYS
1	A	255	LYS
1	A	258[A]	GLN
1	A	258[B]	GLN
1	A	279	LYS
1	A	286	VAL
1	A	289	SER
1	A	321	LYS
1	A	322	ASP
1	A	327	THR
1	A	339	GLU
1	A	340	ILE
1	A	345	ILE
1	A	354	ILE
1	A	355	GLU
1	A	365	LYS
1	B	2	LYS
1	B	8	PHE
1	B	19	ILE
1	B	44	GLU
1	B	47	ASP
1	B	50	ASN
1	B	59	ASN
1	B	69	LYS
1	B	94	SER

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Mol	Chain	Res	Type
1	B	101	ILE
1	B	107	ILE
1	B	108	ARG
1	B	115	SER
1	B	116	LEU
1	B	119	SER
1	B	122	THR
1	B	123	GLU
1	B	128	ILE
1	B	136	GLN
1	B	143	ILE
1	B	150	TYR
1	B	209	LYS
1	B	217	GLU
1	B	223	ILE
1	B	244	LYS
1	B	248	LYS
1	B	252	GLU
1	B	255	LYS
1	B	261	ILE
1	B	266	ASN
1	B	268	ASN
1	B	271	ILE
1	B	274	GLU
1	B	284	THR
1	B	286	VAL
1	B	287	ILE
1	B	290	GLU
1	B	291	LYS
1	B	292	ARG
1	B	294	GLU
1	B	297	LYS
1	B	301	ASN
1	B	307	LEU
1	B	314	ILE
1	B	321	LYS
1	B	322	ASP
1	B	323	LEU
1	B	327	THR
1	B	329	ASN
1	B	335	LYS
1	B	339	GLU

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Mol	Chain	Res	Type
1	B	340	ILE
1	B	342	SER
1	B	345	ILE
1	B	352	GLU
1	B	357	VAL
1	B	360	LYS
1	B	361	ILE

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

Mol	Chain	Res	Type
1	A	265	ASN
1	A	301	ASN
1	B	50	ASN
1	B	65	HIS
1	B	136	GLN
1	B	213	ASN
1	B	222	HIS
1	B	265	ASN
1	B	268	ASN
1	B	338	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	TQP	B	374	-	52,53,53	1.17	4 (7%)	75,81,81	2.04	18 (24%)
2	TQP	A	374	-	52,53,53	1.26	5 (9%)	75,81,81	2.29	19 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TQP	B	374	-	-	7/32/64/64	0/4/4/4
2	TQP	A	374	-	-	12/32/64/64	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	374	TQP	PA-O2A	3.56	1.63	1.50
2	A	374	TQP	PA-O2A	3.46	1.62	1.50
2	B	374	TQP	PB-O2B	2.85	1.60	1.50
2	B	374	TQP	PA-O3A	2.73	1.62	1.59
2	A	374	TQP	PB-O3A	2.72	1.62	1.59
2	B	374	TQP	C2-N1	-2.72	1.34	1.38
2	A	374	TQP	C4-N3	-2.71	1.33	1.38
2	A	374	TQP	C2-N1	-2.55	1.34	1.38
2	A	374	TQP	PB-O2B	2.24	1.58	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	374	TQP	C3Q-N3Q-C4'	7.43	131.12	118.19
2	A	374	TQP	O5'-C5H-C4H	6.87	132.39	108.99
2	B	374	TQP	C4P-C4'-N3Q	-6.61	109.75	122.73
2	A	374	TQP	N3-C2-N1	6.20	122.97	114.89
2	A	374	TQP	C4-N3-C2	-5.86	119.65	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	374	TQP	C4-N3-C2	-5.43	120.22	127.34
2	B	374	TQP	N3-C2-N1	4.63	120.92	114.89
2	A	374	TQP	C5-C6-N1	-4.53	118.39	123.31
2	B	374	TQP	C5-C4-N3	4.52	119.25	115.32
2	B	374	TQP	C3Q-N3Q-C4'	4.42	125.89	118.19
2	A	374	TQP	O2-C2-N1	-4.24	117.28	122.80
2	A	374	TQP	C1Q-O5Q-C5Q	-4.22	106.44	113.63
2	B	374	TQP	C1Q-O5Q-C5Q	-4.22	106.44	113.63
2	B	374	TQP	C6Q-C5Q-C4Q	-4.08	105.62	113.08
2	B	374	TQP	C5-C6-N1	-3.77	119.22	123.31
2	A	374	TQP	C5-C4-N3	3.77	118.60	115.32
2	B	374	TQP	O5'-C5H-C4H	-3.62	96.68	108.99
2	A	374	TQP	O5Q-C5Q-C6Q	3.54	114.59	106.74
2	A	374	TQP	C4Q-C3Q-N3Q	3.45	113.53	109.73
2	B	374	TQP	O4-C4-C5	-3.23	121.22	124.92
2	B	374	TQP	O2-C2-N1	-3.11	118.74	122.80
2	A	374	TQP	C5M-C5-C6	-3.04	118.73	122.85
2	B	374	TQP	PB-O3B-C1Q	-2.82	109.73	121.21
2	A	374	TQP	O3A-PB-O2B	2.81	119.17	110.70
2	A	374	TQP	PB-O3B-C1Q	-2.79	109.83	121.21
2	B	374	TQP	O5Q-C1Q-O3B	2.76	114.97	111.36
2	A	374	TQP	C2Q-C3Q-N3Q	2.75	112.75	109.73
2	B	374	TQP	O1A-PA-O3A	-2.58	100.30	107.27
2	A	374	TQP	C6-C5-C4	2.57	120.14	118.02
2	B	374	TQP	O3B-C1Q-C2Q	2.49	112.95	108.38
2	A	374	TQP	O4'-C4H-C5H	-2.46	101.47	109.33
2	B	374	TQP	O3B-PB-O2B	2.33	117.24	109.81
2	A	374	TQP	O3P-P-O4P	2.26	112.56	106.67
2	A	374	TQP	C5M-C5-C4	2.20	121.13	118.78
2	B	374	TQP	O1A-PA-O5'	-2.19	97.63	107.57
2	A	374	TQP	O4P-C5'-C5P	2.09	113.27	109.36
2	B	374	TQP	C2H-C3'-C4H	2.06	106.98	102.80

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	374	TQP	C4H-C5H-O5'-PA
2	A	374	TQP	C5H-O5'-PA-O2A
2	A	374	TQP	C4Q-C3Q-N3Q-C4'
2	B	374	TQP	C5H-O5'-PA-O2A
2	B	374	TQP	C4Q-C3Q-N3Q-C4'

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Mol	Chain	Res	Type	Atoms
2	A	374	TQP	C4P-C4'-N3Q-C3Q
2	A	374	TQP	O4'-C4H-C5H-O5'
2	A	374	TQP	C3'-C4H-C5H-O5'
2	B	374	TQP	C2Q-C1Q-O3B-PB
2	A	374	TQP	C1Q-O3B-PB-O2B
2	B	374	TQP	C5'-O4P-P-O1P
2	A	374	TQP	C2Q-C1Q-O3B-PB
2	A	374	TQP	PB-O3A-PA-O5'
2	B	374	TQP	C5'-O4P-P-O2P
2	B	374	TQP	C1Q-O3B-PB-O2B
2	A	374	TQP	PA-O3A-PB-O2B
2	B	374	TQP	N3Q-C4'-C4P-C3P
2	A	374	TQP	PB-O3A-PA-O1A
2	A	374	TQP	PA-O3A-PB-O1B

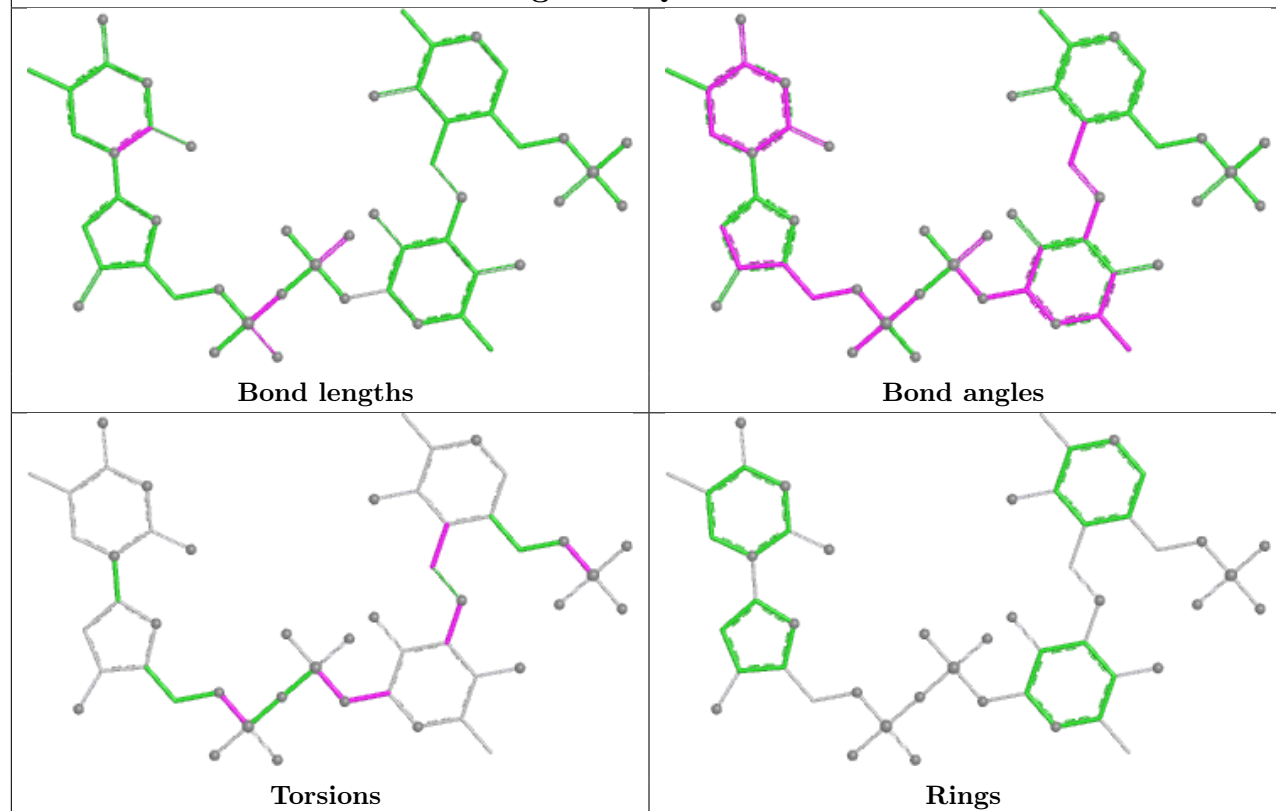
There are no ring outliers.

2 monomers are involved in 7 short contacts:

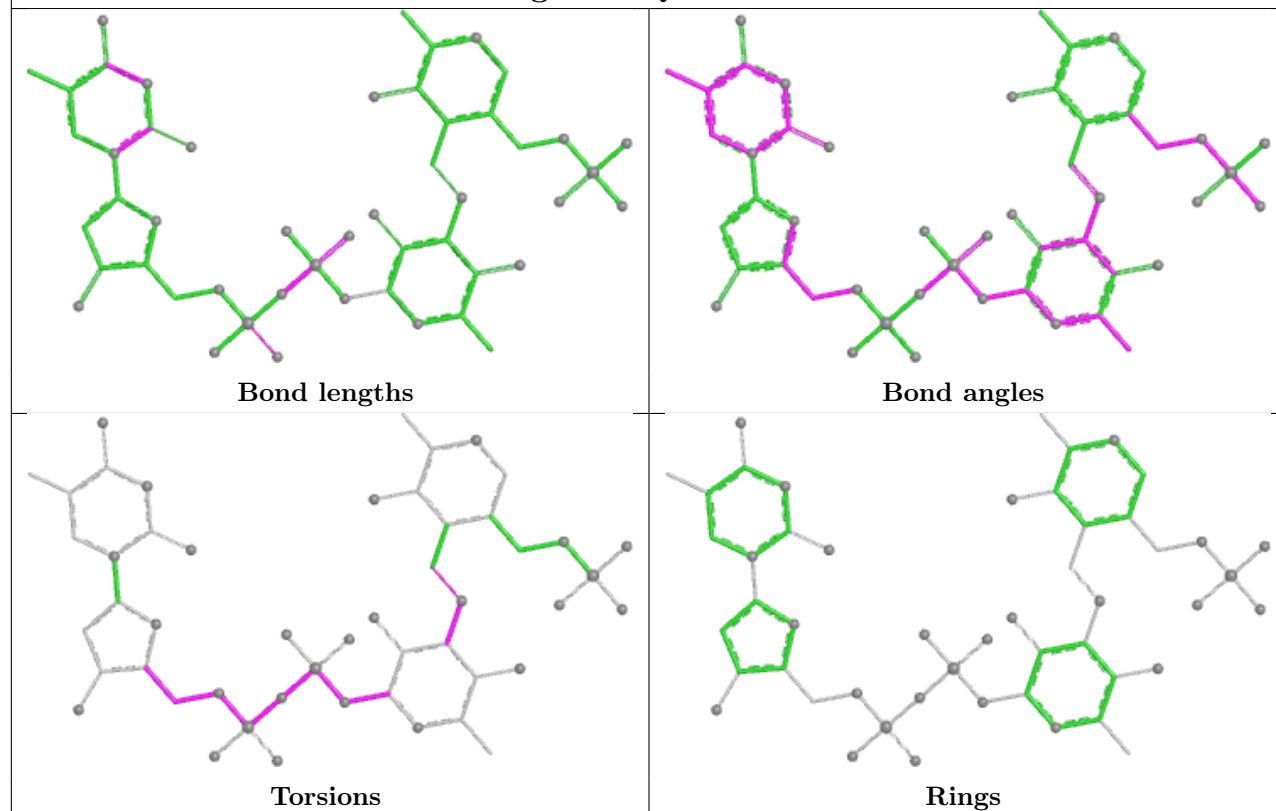
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	374	TQP	4	0
2	A	374	TQP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand TQP B 374



Ligand TQP A 374



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	A	365/373 (97%)	-0.33	0 100 100	24, 43, 72, 88	3 (0%)
1	B	364/373 (97%)	-0.30	0 100 100	25, 52, 77, 97	1 (0%)
All	All	729/746 (97%)	-0.32	0 100 100	24, 48, 75, 97	4 (0%)

There are no RSRZ outliers to report.

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](#)

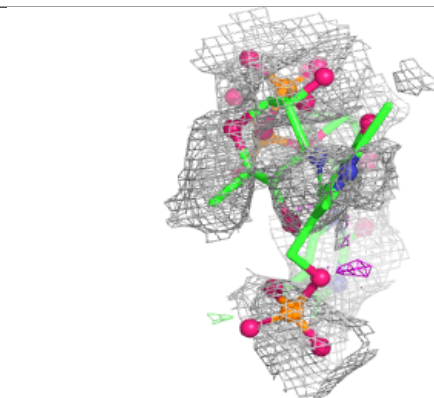
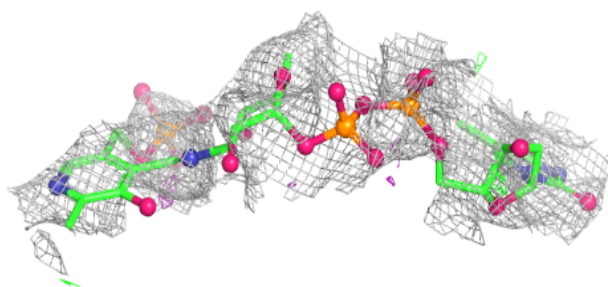
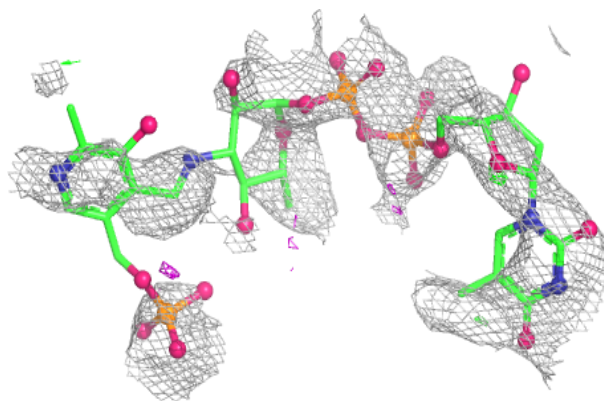
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TQP	B	374	50/50	0.90	0.07	21,48,100,100	0
2	TQP	A	374	50/50	0.93	0.07	18,36,72,86	0

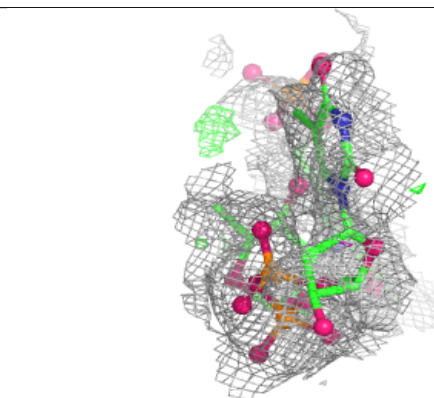
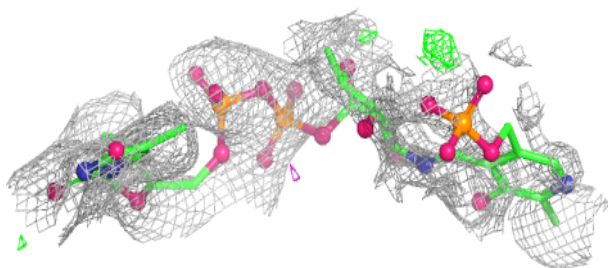
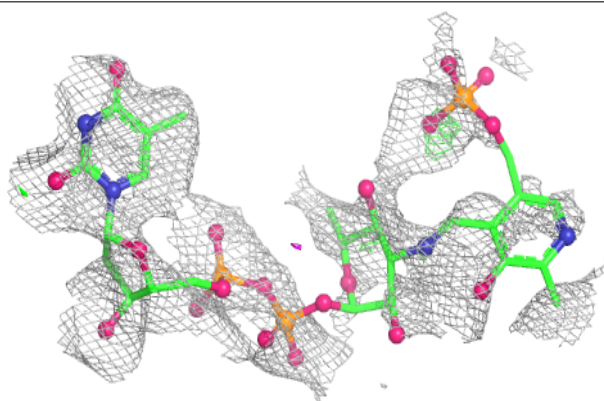
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TQP B 374:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TQP A 374:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.