



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:58 PM UTC

PDB ID : 1JLC / pdb_00001jlc
Title : CRYSTAL STRUCTURE OF Y181C MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH PETT-2
Authors : Ren, J.; Nichols, C.; Bird, L.; Chamberlain, P.; Weaver, K.; Short, S.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2001-07-16
Resolution : 3.00 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
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

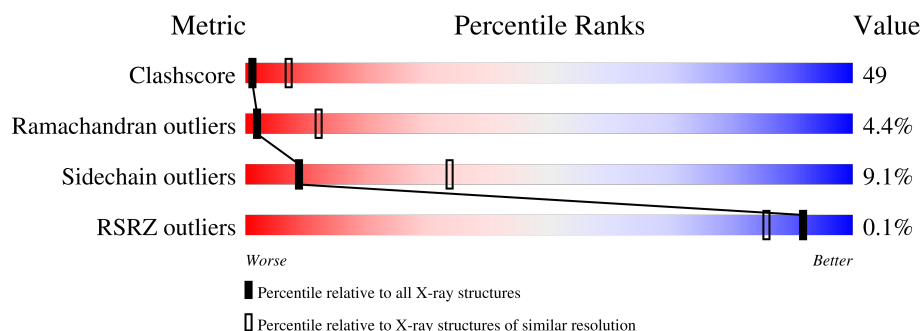
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

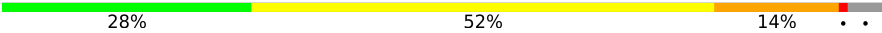
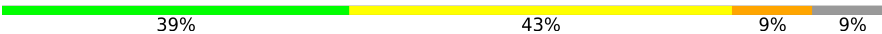
The reported resolution of this entry is 3.00 Å.

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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	560	
2	B	440	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7711 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 HIV-1 RT A-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4361	2821	726	805	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	CYS	TYR	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

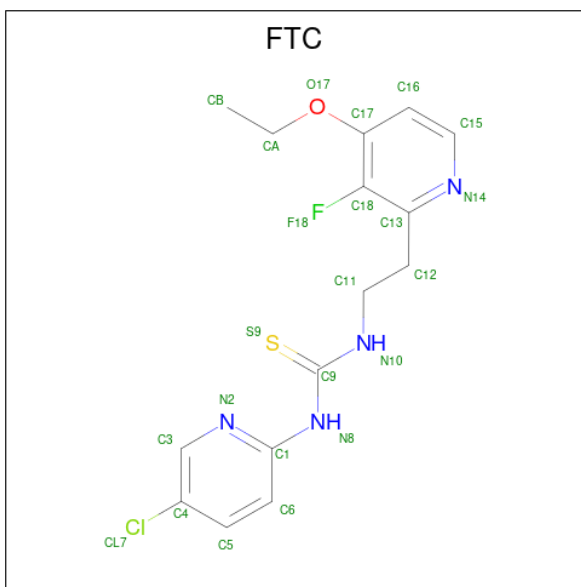
- Molecule 2 is a protein called HIV-1 RT B-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3327	2158	555	606	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	181	CYS	TYR	engineered mutation	UNP P04585

- Molecule 3 is N-[[3-FLUORO-4-ETHOXY-PYRID-2-YL]ETHYL]-N'-[5-CHLORO-PYRIDYL]-THIOUREA (CCD ID: FTC) (formula: C₁₅H₁₆ClFN₄OS).

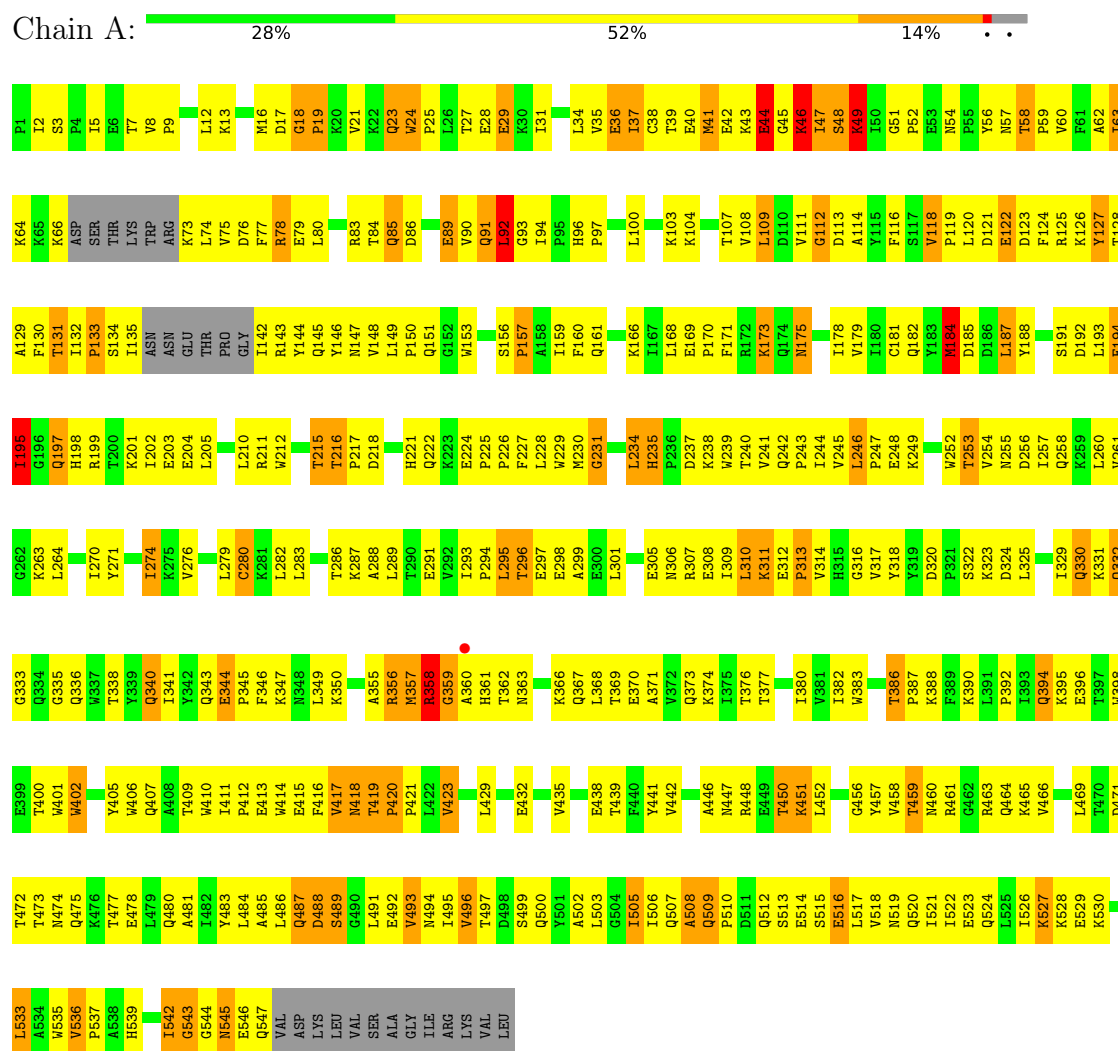


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	F	N	O	S		
3	A	1	23	15	1	1	4	1	1	0	0

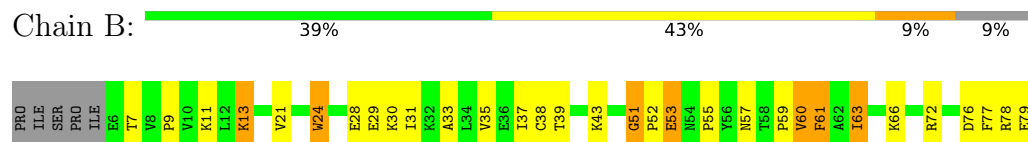
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: HIV-1 RT A-chain



• Molecule 2: HIV-1 RT B-chain



D86	Q155	Q156	Q157	Q158	Q159	Q160	Q161	Q162	Q163	Q164	Q165	Q166	Q167	Q168	Q169	Q170	Q171	Q172	Q173	Q174	Q175	Q176	Q177	Q178	Q179	Q180	Q181	Q182	Q183	Q184	Q185	Q186	Q187	Q188	Q189	Q190	Q191	Q192	Q193	Q194	Q195	Q196	Q197	Q198	Q199	Q200	Q201	Q202	Q203	Q204	Q205	Q206	Q207	Q208	Q209	Q210	Q211	Q212	Q213	Q214	Q215	Q216	Q217	Q218	Q219	Q220	Q221	Q222	Q223	Q224	Q225	Q226	Q227	Q228	Q229	Q230	Q231	Q232	Q233	Q234	Q235	Q236	Q237	Q238	Q239	Q240	Q241	Q242	Q243	Q244	Q245	Q246	Q247	Q248	Q249	Q250	Q251	Q252	Q253	Q254	Q255	Q256	Q257	Q258	Q259	Q260	Q261	Q262	Q263	Q264	Q265	Q266	Q267	Q268	Q269	Q270	Q271	Q272	Q273	Q274	Q275	Q276	Q277	Q278	Q279	Q280	Q281	Q282	Q283	Q284	Q285	Q286	Q287	Q288	Q289	Q290	Q291	Q292	Q293	Q294	Q295	Q296	Q297	Q298	Q299	Q300	Q301	Q302	Q303	Q304	Q305	Q306	Q307	Q308	Q309	Q310	Q311	Q312	Q313	Q314	Q315	Q316	Q317	Q318	Q319	Q320	Q321	Q322	Q323	Q324	Q325	Q326	Q327	Q328	Q329	Q330	Q331	Q332	Q333	Q334	Q335	Q336	Q337	Q338	Q339	Q340	Q341	Q342	Q343	Q344	Q345	Q346	Q347	Q348	Q349	Q350	Q351	Q352	Q353	Q354	Q355	Q356	Q357	Q358	Q359	Q360	Q361	Q362	Q363	Q364	Q365	Q366	Q367	Q368	Q369	Q370	Q371	Q372	Q373	Q374	Q375	Q376	Q377	Q378	Q379	Q380	Q381	Q382	Q383	Q384	Q385	Q386	Q387	Q388	Q389	Q390	Q391	Q392	Q393	Q394	Q395	Q396	Q397	Q398	Q399	Q400	Q401	Q402	Q403	Q404	Q405	Q406	Q407	Q408	Q409	Q410	Q411	Q412	Q413	Q414	Q415	Q416	Q417	Q418	Q419	Q420	Q421	Q422	Q423	Q424	Q425	Q426	Q427	Q428	Q429	Q430	Q431	Q432	Q433	Q434	Q435	Q436	Q437	Q438	Q439	Q440	Q441	Q442	Q443	Q444	Q445	Q446	Q447	Q448	Q449	Q450	Q451	Q452	Q453	Q454	Q455	Q456	Q457	Q458	Q459	Q460	Q461	Q462	Q463	Q464	Q465	Q466	Q467	Q468	Q469	Q470	Q471	Q472	Q473	Q474	Q475	Q476	Q477	Q478	Q479	Q480	Q481	Q482	Q483	Q484	Q485	Q486	Q487	Q488	Q489	Q490	Q491	Q492	Q493	Q494	Q495	Q496	Q497	Q498	Q499	Q500	Q501	Q502	Q503	Q504	Q505	Q506	Q507	Q508	Q509	Q510	Q511	Q512	Q513	Q514	Q515	Q516	Q517	Q518	Q519	Q520	Q521	Q522	Q523	Q524	Q525	Q526	Q527	Q528	Q529	Q530	Q531	Q532	Q533	Q534	Q535	Q536	Q537	Q538	Q539	Q540	Q541	Q542	Q543	Q544	Q545	Q546	Q547	Q548	Q549	Q550	Q551	Q552	Q553	Q554	Q555	Q556	Q557	Q558	Q559	Q560	Q561	Q562	Q563	Q564	Q565	Q566	Q567	Q568	Q569	Q570	Q571	Q572	Q573	Q574	Q575	Q576	Q577	Q578	Q579	Q580	Q581	Q582	Q583	Q584	Q585	Q586	Q587	Q588	Q589	Q590	Q591	Q592	Q593	Q594	Q595	Q596	Q597	Q598	Q599	Q600	Q601	Q602	Q603	Q604	Q605	Q606	Q607	Q608	Q609	Q610	Q611	Q612	Q613	Q614	Q615	Q616	Q617	Q618	Q619	Q620	Q621	Q622	Q623	Q624	Q625	Q626	Q627	Q628	Q629	Q630	Q631	Q632	Q633	Q634	Q635	Q636	Q637	Q638	Q639	Q640	Q641	Q642	Q643	Q644	Q645	Q646	Q647	Q648	Q649	Q650	Q651	Q652	Q653	Q654	Q655	Q656	Q657	Q658	Q659	Q660	Q661	Q662	Q663	Q664	Q665	Q666	Q667	Q668	Q669	Q670	Q671	Q672	Q673	Q674	Q675	Q676	Q677	Q678	Q679	Q680	Q681	Q682	Q683	Q684	Q685	Q686	Q687	Q688	Q689	Q690	Q691	Q692	Q693	Q694	Q695	Q696	Q697	Q698	Q699	Q700	Q701	Q702	Q703	Q704	Q705	Q706	Q707	Q708	Q709	Q710	Q711	Q712	Q713	Q714	Q715	Q716	Q717	Q718	Q719	Q720	Q721	Q722	Q723	Q724	Q725	Q726	Q727	Q728	Q729	Q730	Q731	Q732	Q733	Q734	Q735	Q736	Q737	Q738	Q739	Q740	Q741	Q742	Q743	Q744	Q745	Q746	Q747	Q748	Q749	Q750	Q751	Q752	Q753	Q754	Q755	Q756	Q757	Q758	Q759	Q760	Q761	Q762	Q763	Q764	Q765	Q766	Q767	Q768	Q769	Q770	Q771	Q772	Q773	Q774	Q775	Q776	Q777	Q778	Q779	Q780	Q781	Q782	Q783	Q784	Q785	Q786	Q787	Q788	Q789	Q790	Q791	Q792	Q793	Q794	Q795	Q796	Q797	Q798	Q799	Q800	Q801	Q802	Q803	Q804	Q805	Q806	Q807	Q808	Q809	Q810	Q811	Q812	Q813	Q814	Q815	Q816	Q817	Q818	Q819	Q820	Q821	Q822	Q823	Q824	Q825	Q826	Q827	Q828	Q829	Q830	Q831	Q832	Q833	Q834	Q835	Q836	Q837	Q838	Q839	Q840	Q841	Q842	Q843	Q844	Q845	Q846	Q847	Q848	Q849	Q850	Q851	Q852	Q853	Q854	Q855	Q856	Q857	Q858	Q859	Q860	Q861	Q862	Q863	Q864	Q865	Q866	Q867	Q868	Q869	Q870	Q871	Q872	Q873	Q874	Q875	Q876	Q877	Q878	Q879	Q880	Q881	Q882	Q883	Q884	Q885	Q886	Q887	Q888	Q889	Q890	Q891	Q892	Q893	Q894	Q895	Q896	Q897	Q898	Q899	Q900	Q901	Q902	Q903	Q904	Q905	Q906	Q907	Q908	Q909	Q910	Q911	Q912	Q913	Q914	Q915	Q916	Q917	Q918	Q919	Q920	Q921	Q922	Q923	Q924	Q925	Q926	Q927	Q928	Q929	Q930	Q931	Q932	Q933	Q934	Q935	Q936	Q937	Q938	Q939	Q940	Q941	Q942	Q943	Q944	Q945	Q946	Q947	Q948	Q949	Q950	Q951	Q952	Q953	Q954	Q955	Q956	Q957	Q958	Q959	Q960	Q961	Q962	Q963	Q964	Q965	Q966	Q967	Q968	Q969	Q970	Q971	Q972	Q973	Q974	Q975	Q976	Q977	Q978	Q979	Q980	Q981	Q982	Q983	Q984	Q985	Q986	Q987	Q988	Q989	Q990	Q991	Q992	Q993	Q994	Q995	Q996	Q997	Q998	Q999	Q1000	Q1001	Q1002	Q1003	Q1004	Q1005	Q1006	Q1007	Q1008	Q1009	Q1010	Q1011	Q1012	Q1013	Q1014	Q1015	Q1016	Q1017	Q1018	Q1019	Q1020	Q1021	Q1022	Q1023	Q1024	Q1025	Q1026	Q1027	Q1028	Q1029	Q1030	Q1031	Q1032	Q1033	Q1034	Q1035	Q1036	Q1037	Q1038	Q1039	Q1040	Q1041	Q1042	Q1043	Q1044	Q1045	Q1046	Q1047	Q1048	Q1049	Q1050	Q1051	Q1052	Q1053	Q1054	Q1055	Q1056	Q1057	Q1058	Q1059	Q1060	Q1061	Q1062	Q1063	Q1064	Q1065	Q1066	Q1067	Q1068	Q1069	Q1070	Q1071	Q1072	Q1073	Q1074	Q1075	Q1076	Q1077	Q1078	Q1079	Q1080	Q1081	Q1082	Q1083	Q1084	Q1085	Q1086	Q1087	Q1088	Q1089	Q1090	Q1091	Q1092	Q1093	Q1094	Q1095	Q1096	Q1097	Q1098	Q1099	Q1100	Q1101	Q1102	Q1103	Q1104	Q1105	Q1106	Q1107	Q1108	Q1109	Q1110	Q1111	Q1112	Q1113	Q1114	Q1115	Q1116	Q1117	Q1118	Q1119	Q1120	Q1121	Q1122	Q1123	Q1124	Q1125	Q1126	Q1127	Q11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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	139.20Å 109.30Å 73.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 3.00 29.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.79-3.00) 96.9 (29.79-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.282 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 84.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7711	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: FTC, CSD

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	0.67	0/4464	1.18	39/6061 (0.6%)
2	B	0.66	0/3418	1.14	30/4638 (0.6%)
All	All	0.67	0/7882	1.16	69/10699 (0.6%)

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

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

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	356	ARG	N-CA-C	13.10	127.27	110.24
2	B	87	PHE	CA-C-N	-9.57	109.69	122.42
2	B	87	PHE	C-N-CA	-9.57	109.69	122.42
2	B	131	THR	N-CA-C	9.25	123.51	108.34
1	A	175	ASN	CA-C-N	9.03	129.21	119.28
1	A	175	ASN	C-N-CA	9.03	129.21	119.28
1	A	358	ARG	N-CA-C	8.45	119.40	108.24
2	B	343	GLN	N-CA-C	-8.32	103.32	113.97
2	B	417	VAL	N-CA-C	7.91	118.19	108.53
1	A	235	HIS	CA-C-N	7.83	127.49	119.82
1	A	235	HIS	C-N-CA	7.83	127.49	119.82
1	A	234	LEU	N-CA-C	7.66	121.72	109.24
1	A	51	GLY	CA-C-N	7.41	129.10	119.84
1	A	51	GLY	C-N-CA	7.41	129.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	GLU	N-CA-C	-7.34	103.22	111.07
2	B	326	ILE	N-CA-C	7.14	118.88	108.53
1	A	118	VAL	N-CA-C	7.13	116.46	108.05
2	B	349	LEU	N-CA-C	-7.02	104.84	113.41
1	A	349	LEU	N-CA-C	-7.00	103.38	112.68
1	A	388	LYS	N-CA-C	-6.96	99.20	110.20
1	A	37	ILE	N-CA-C	-6.95	106.27	111.90
2	B	147	ASN	N-CA-C	-6.95	105.34	114.31
1	A	184	MET	CB-CA-C	-6.90	108.62	116.63
1	A	493	VAL	N-CA-C	6.88	118.63	108.45
2	B	135	ILE	N-CA-C	6.75	118.28	109.58
1	A	509	GLN	CA-C-N	-6.71	113.05	119.76
1	A	509	GLN	C-N-CA	-6.71	113.05	119.76
2	B	428	GLN	N-CA-C	-6.65	104.07	111.71
1	A	539	HIS	N-CA-C	6.60	120.66	112.47
1	A	18	GLY	CA-C-N	6.50	127.96	119.84
1	A	18	GLY	C-N-CA	6.50	127.96	119.84
1	A	58	THR	CA-C-N	6.46	126.48	119.90
1	A	58	THR	C-N-CA	6.46	126.48	119.90
2	B	235	HIS	CA-C-N	6.43	126.93	119.47
2	B	235	HIS	C-N-CA	6.43	126.93	119.47
1	A	355	ALA	N-CA-C	6.40	118.61	110.61
2	B	115	TYR	N-CA-C	6.38	119.05	111.33
2	B	86	ASP	N-CA-C	-6.23	101.72	110.50
2	B	24	TRP	N-CA-C	-6.21	101.18	110.24
2	B	401	TRP	N-CA-C	6.12	122.34	114.56
2	B	13	LYS	N-CA-C	-6.09	101.38	109.84
1	A	402	TRP	N-CA-C	6.07	118.68	111.33
2	B	307	ARG	N-CA-C	-6.07	104.58	111.07
2	B	366	LYS	N-CA-C	-5.88	104.56	110.97
1	A	211	ARG	N-CA-C	-5.83	106.51	113.21
2	B	171	PHE	N-CA-C	-5.79	106.86	114.04
1	A	359	GLY	N-CA-C	-5.79	105.84	112.79
1	A	224	GLU	N-CA-C	5.74	118.58	109.40
1	A	297	GLU	N-CA-C	-5.73	105.03	111.28
2	B	186	ASP	N-CA-C	5.73	119.40	110.17
2	B	98	ALA	N-CA-C	-5.59	106.13	113.17
1	A	49	LYS	N-CA-C	-5.55	98.98	110.80
2	B	370	GLU	N-CA-C	-5.52	104.28	111.02
2	B	414	TRP	N-CA-C	5.47	117.59	108.99
1	A	527	LYS	N-CA-C	5.46	117.99	111.71
2	B	172	ARG	N-CA-C	-5.41	105.54	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	88	TRP	CA-CB-CG	-5.27	103.58	113.60
1	A	528	LYS	N-CA-C	5.27	117.67	110.55
1	A	371	ALA	N-CA-C	-5.22	105.49	111.07
1	A	231	GLY	N-CA-C	-5.16	108.00	115.27
2	B	202	ILE	N-CA-C	-5.13	105.60	110.42
1	A	344	GLU	N-CA-C	-5.12	102.19	109.62
2	B	83	ARG	N-CA-C	5.09	119.55	113.23
1	A	48	SER	N-CA-C	-5.08	99.97	110.80
1	A	195	ILE	N-CA-C	5.08	119.91	109.34
2	B	51	GLY	CA-C-N	5.02	124.63	119.56
2	B	51	GLY	C-N-CA	5.02	124.63	119.56
1	A	46	LYS	N-CA-C	5.01	121.48	110.80
1	A	133	PRO	N-CA-C	5.00	119.05	110.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4361	0	4413	528	0
2	B	3327	0	3352	249	0
3	A	23	0	16	4	0
All	All	7711	0	7781	761	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 49.

All (761) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:H	1:A:228:LEU:HD23	1.04	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:HB3	1:A:47:ILE:HD13	1.25	1.13
1:A:216:THR:HG22	1:A:217:PRO:HD2	1.28	1.09
1:A:41:MET:HG2	1:A:46:LYS:HD2	1.32	1.09
1:A:41:MET:HB3	1:A:47:ILE:CD1	1.86	1.05
2:B:98:ALA:HA	2:B:101:LYS:HD3	1.40	1.03
1:A:536:VAL:HG21	1:A:542:ILE:HG21	1.38	1.02
1:A:274:ILE:HD11	1:A:310:LEU:HD11	1.43	1.01
1:A:46:LYS:HB3	1:A:47:ILE:HD12	1.40	1.01
1:A:244:ILE:HD11	1:A:263:LYS:HD3	1.39	0.99
1:A:47:ILE:HG21	1:A:144:TYR:HB3	1.46	0.97
1:A:132:ILE:HB	1:A:142:ILE:HG22	1.48	0.95
1:A:123:ASP:O	1:A:126:LYS:HD3	1.67	0.95
1:A:491:LEU:HB3	1:A:529:GLU:HB2	1.50	0.94
1:A:418:ASN:O	1:A:420:PRO:HD3	1.67	0.93
1:A:358:ARG:NH2	1:A:514:GLU:N	2.18	0.92
1:A:417:VAL:HG12	1:A:419:THR:HG22	1.52	0.92
1:A:228:LEU:H	1:A:228:LEU:CD2	1.80	0.92
1:A:499:SER:HB2	1:A:502:ALA:HB3	1.51	0.92
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.69	0.91
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.54	0.90
1:A:358:ARG:HH22	1:A:514:GLU:N	1.67	0.90
1:A:75:VAL:HG12	1:A:76:ASP:H	1.32	0.90
1:A:120:LEU:HD12	1:A:121:ASP:H	1.33	0.90
1:A:356:ARG:HH22	1:A:374:LYS:HZ1	1.15	0.90
2:B:263:LYS:HE2	2:B:425:LEU:HB3	1.52	0.89
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.54	0.89
1:A:356:ARG:HH22	1:A:374:LYS:NZ	1.71	0.89
1:A:447:ASN:HB3	1:A:450:THR:HG23	1.54	0.89
1:A:46:LYS:HE3	1:A:116:PHE:CD2	2.08	0.89
1:A:356:ARG:HH12	1:A:374:LYS:HZ3	1.21	0.88
1:A:130:PHE:HB2	1:A:144:TYR:H	1.38	0.88
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.08	0.88
1:A:41:MET:HG2	1:A:46:LYS:CD	2.04	0.87
1:A:228:LEU:HD23	1:A:228:LEU:N	1.90	0.86
1:A:47:ILE:HG23	1:A:145:GLN:O	1.78	0.84
2:B:175:ASN:HD21	2:B:201:LYS:HZ1	1.26	0.84
1:A:47:ILE:CG2	1:A:144:TYR:HB3	2.08	0.83
1:A:47:ILE:HG22	1:A:48:SER:N	1.92	0.83
1:A:57:ASN:HD22	1:A:58:THR:H	1.24	0.83
1:A:523:GLU:HB3	1:A:527:LYS:NZ	1.94	0.81
1:A:130:PHE:CD1	1:A:144:TYR:HB2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:GLU:C	2:B:234:LEU:HD12	2.05	0.81
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.63	0.81
1:A:57:ASN:HD22	1:A:58:THR:N	1.79	0.80
1:A:390:LYS:HE2	1:A:415:GLU:OE2	1.82	0.80
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.63	0.79
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.18	0.79
2:B:98:ALA:HA	2:B:101:LYS:CD	2.12	0.79
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.46	0.78
1:A:41:MET:CB	1:A:47:ILE:HD13	2.11	0.78
2:B:109:LEU:HB2	2:B:187:LEU:HB3	1.63	0.78
1:A:296:THR:HG22	1:A:298:GLU:OE2	1.84	0.78
1:A:356:ARG:NH2	1:A:374:LYS:HZ1	1.83	0.77
2:B:98:ALA:CA	2:B:101:LYS:HD3	2.12	0.76
2:B:119:PRO:HA	2:B:148:VAL:HA	1.67	0.76
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.13	0.76
1:A:75:VAL:HG12	1:A:76:ASP:N	2.00	0.76
1:A:358:ARG:HD3	1:A:512:GLN:HG3	1.66	0.76
2:B:163:SER:HA	2:B:166:LYS:HE2	1.67	0.75
1:A:370:GLU:O	1:A:374:LYS:HG3	1.86	0.75
1:A:210:LEU:CD1	1:A:215:THR:HA	2.16	0.74
1:A:283:LEU:O	1:A:286:THR:HG23	1.86	0.74
2:B:242:GLN:HB2	2:B:430:GLU:OE1	1.87	0.74
1:A:235:HIS:HB2	1:A:238:LYS:HG3	1.68	0.74
1:A:2:ILE:HD11	1:A:45:GLY:HA3	1.70	0.74
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.70	0.74
1:A:23:GLN:HG2	1:A:131:THR:CG2	2.18	0.74
2:B:89:GLU:O	2:B:89:GLU:HG2	1.87	0.74
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.70	0.74
1:A:37:ILE:HD13	1:A:73:LYS:HB2	1.68	0.73
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.70	0.73
1:A:56:TYR:O	1:A:129:ALA:HB3	1.88	0.73
1:A:335:GLY:HA2	1:A:367:GLN:OE1	1.89	0.73
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.70	0.73
1:A:452:LEU:HA	1:A:469:LEU:O	1.87	0.73
2:B:239:TRP:HZ3	2:B:382:ILE:HD11	1.53	0.73
2:B:206:ARG:O	2:B:210:LEU:HD13	1.88	0.72
1:A:356:ARG:HH22	1:A:374:LYS:CE	2.02	0.72
1:A:23:GLN:HG2	1:A:131:THR:HG21	1.71	0.72
2:B:31:ILE:O	2:B:35:VAL:HG23	1.90	0.72
1:A:358:ARG:NH2	1:A:513:SER:C	2.47	0.72
1:A:57:ASN:ND2	1:A:58:THR:N	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD12	1:A:47:ILE:N	2.05	0.71
1:A:47:ILE:HG22	1:A:48:SER:H	1.53	0.71
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.70	0.71
1:A:125:ARG:HB3	1:A:146:TYR:O	1.91	0.71
1:A:243:PRO:HG3	1:A:313:PRO:CG	2.21	0.71
1:A:170:PRO:HG2	1:A:171:PHE:H	1.55	0.71
2:B:266:TRP:CD1	2:B:267:ALA:N	2.58	0.71
1:A:5:ILE:HD11	1:A:166:LYS:HE3	1.73	0.71
1:A:465:LYS:NZ	1:A:488:ASP:OD2	2.24	0.71
2:B:296:THR:HG22	2:B:298:GLU:OE1	1.91	0.71
1:A:39:THR:O	1:A:42:GLU:HG2	1.91	0.71
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.73	0.71
1:A:418:ASN:C	1:A:420:PRO:HD3	2.15	0.70
1:A:457:TYR:HE2	1:A:465:LYS:HD2	1.56	0.70
2:B:358:ARG:H	2:B:358:ARG:HD3	1.55	0.70
1:A:66:LYS:H	1:A:66:LYS:HD2	1.56	0.70
1:A:120:LEU:HD12	1:A:121:ASP:N	2.07	0.70
2:B:332:GLN:HB2	2:B:336:GLN:HB3	1.73	0.70
1:A:451:LYS:HB3	1:A:472:THR:N	2.06	0.69
1:A:118:VAL:O	1:A:148:VAL:HG22	1.93	0.69
1:A:358:ARG:CD	1:A:512:GLN:HG3	2.21	0.69
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.22	0.69
1:A:317:VAL:HG22	1:A:318:TYR:H	1.58	0.69
1:A:485:ALA:O	1:A:489:SER:HB3	1.92	0.69
2:B:420:PRO:O	2:B:423:VAL:HG22	1.93	0.69
1:A:331:LYS:HG2	1:A:333:GLY:O	1.92	0.69
1:A:246:LEU:O	1:A:307:ARG:NH1	2.26	0.69
1:A:516:GLU:HG3	1:A:517:LEU:N	2.08	0.69
1:A:122:GLU:H	1:A:122:GLU:CD	2.02	0.68
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.28	0.68
2:B:233:GLU:O	2:B:234:LEU:HD12	1.94	0.68
2:B:425:LEU:O	2:B:429:LEU:HD13	1.93	0.68
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.75	0.68
1:A:35:VAL:O	1:A:39:THR:HG23	1.93	0.68
1:A:114:ALA:HB1	1:A:160:PHE:HE2	1.59	0.67
1:A:254:VAL:CG2	1:A:291:GLU:HB3	2.24	0.67
2:B:194:GLU:HG2	2:B:195:ILE:N	2.07	0.67
2:B:296:THR:HG22	2:B:298:GLU:H	1.58	0.67
1:A:210:LEU:C	1:A:212:TRP:H	2.03	0.67
2:B:278:GLN:HA	2:B:278:GLN:NE2	2.09	0.67
1:A:435:VAL:HA	2:B:290:THR:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LYS:O	2:B:85:GLN:HG2	1.95	0.67
1:A:90:VAL:O	1:A:91:GLN:HB2	1.94	0.67
1:A:109:LEU:HD12	1:A:109:LEU:N	2.09	0.67
1:A:546:GLU:HG3	1:A:547:GLN:NE2	2.09	0.67
2:B:281:LYS:O	2:B:284:ARG:HG2	1.94	0.67
1:A:132:ILE:HB	1:A:142:ILE:CG2	2.23	0.66
1:A:282:LEU:H	1:A:282:LEU:HD22	1.60	0.66
2:B:422:LEU:HD12	2:B:422:LEU:H	1.60	0.66
1:A:8:VAL:HG21	1:A:159:ILE:HG12	1.77	0.66
1:A:356:ARG:HH12	1:A:374:LYS:NZ	1.92	0.66
1:A:441:TYR:HA	1:A:496:VAL:HG22	1.77	0.66
1:A:362:THR:HG22	1:A:363:ASN:N	2.11	0.66
1:A:500:GLN:HE22	2:B:422:LEU:HD11	1.60	0.66
1:A:47:ILE:HG21	1:A:144:TYR:CB	2.25	0.66
1:A:460:ASN:HD21	1:A:461:ARG:NH1	1.94	0.66
1:A:451:LYS:HB3	1:A:472:THR:H	1.61	0.65
1:A:118:VAL:O	1:A:148:VAL:CG2	2.44	0.65
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.30	0.65
1:A:480:GLN:HE21	1:A:484:LEU:HG	1.61	0.65
1:A:60:VAL:HG11	1:A:73:LYS:HZ1	1.61	0.65
2:B:173:LYS:O	2:B:176:PRO:HD3	1.96	0.65
2:B:389:PHE:HB3	2:B:391:LEU:HD21	1.79	0.65
1:A:188:TYR:HB3	3:A:999:FTC:C18	2.27	0.65
1:A:27:THR:O	1:A:31:ILE:HG12	1.95	0.65
1:A:491:LEU:HB3	1:A:529:GLU:CB	2.26	0.65
1:A:100:LEU:O	1:A:318:TYR:HB3	1.96	0.64
1:A:123:ASP:C	1:A:126:LYS:HD3	2.22	0.64
1:A:118:VAL:HB	1:A:149:LEU:HD13	1.78	0.64
1:A:518:VAL:O	1:A:522:ILE:HG13	1.97	0.64
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.32	0.64
1:A:254:VAL:HB	1:A:289:LEU:O	1.98	0.64
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.64
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.32	0.64
1:A:96:HIS:CD2	1:A:230:MET:HE1	2.32	0.64
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.13	0.64
1:A:366:LYS:O	1:A:369:THR:HB	1.98	0.64
1:A:31:ILE:HD12	1:A:133:PRO:O	1.97	0.64
1:A:500:GLN:NE2	2:B:422:LEU:HD11	2.12	0.64
1:A:225:PRO:HA	1:A:226:PRO:C	2.24	0.63
1:A:330:GLN:HG2	1:A:338:THR:OG1	1.97	0.63
1:A:362:THR:HG22	1:A:363:ASN:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLN:OE1	2:B:422:LEU:HD11	1.99	0.63
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.33	0.63
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.34	0.63
1:A:451:LYS:O	1:A:471:ASP:N	2.30	0.63
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.29	0.63
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.34	0.63
1:A:513:SER:HB3	1:A:519:ASN:ND2	2.13	0.63
1:A:47:ILE:CG2	1:A:48:SER:N	2.59	0.63
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.79	0.63
1:A:37:ILE:O	1:A:40:GLU:HB3	1.99	0.62
2:B:183:TYR:CE1	2:B:184:MET:HE2	2.34	0.62
2:B:239:TRP:CZ3	2:B:382:ILE:HD11	2.34	0.62
1:A:73:LYS:HD3	1:A:74:LEU:H	1.64	0.62
1:A:104:LYS:HD2	1:A:192:ASP:O	1.99	0.62
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.33	0.62
1:A:181:CYS:HB2	2:B:138:GLU:OE2	1.99	0.62
1:A:249:LYS:HB3	1:A:252:TRP:CE2	2.34	0.62
1:A:332:GLN:HG3	1:A:338:THR:CG2	2.28	0.62
1:A:438:GLU:OE1	1:A:459:THR:HG21	1.98	0.62
1:A:473:THR:O	1:A:477:THR:HG23	1.99	0.62
1:A:500:GLN:HE22	2:B:422:LEU:HD21	1.63	0.62
1:A:358:ARG:NH2	1:A:513:SER:HA	2.15	0.62
1:A:47:ILE:CG2	1:A:48:SER:H	2.12	0.62
1:A:254:VAL:HG23	1:A:291:GLU:HB3	1.80	0.62
2:B:179:VAL:HG12	2:B:190:GLY:O	2.00	0.62
1:A:60:VAL:HG12	1:A:60:VAL:O	2.00	0.62
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.81	0.62
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.82	0.61
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.82	0.61
1:A:228:LEU:O	1:A:228:LEU:HG	1.99	0.61
2:B:169:GLU:O	2:B:173:LYS:HG2	1.98	0.61
1:A:13:LYS:HE3	1:A:84:THR:O	2.00	0.61
1:A:258:GLN:HE22	1:A:289:LEU:HD11	1.64	0.61
2:B:130:PHE:CE2	2:B:144:TYR:HB2	2.34	0.61
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.30	0.61
2:B:120:LEU:HD23	2:B:121:ASP:N	2.15	0.61
1:A:38:CYS:SG	1:A:73:LYS:HE3	2.40	0.61
1:A:254:VAL:HG21	1:A:288:ALA:O	2.00	0.61
1:A:358:ARG:CZ	1:A:513:SER:HA	2.30	0.61
2:B:163:SER:O	2:B:167:ILE:HG13	2.01	0.61
1:A:407:GLN:HG3	2:B:393:ILE:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:THR:HG21	2:B:153:TRP:NE1	2.16	0.61
1:A:12:LEU:O	1:A:13:LYS:C	2.44	0.60
1:A:75:VAL:CG1	1:A:76:ASP:H	2.10	0.60
2:B:368:LEU:O	2:B:371:ALA:HB3	2.01	0.60
1:A:270:ILE:HG22	1:A:314:VAL:HG21	1.84	0.60
1:A:474:ASN:O	1:A:477:THR:OG1	2.11	0.60
2:B:287:LYS:HD3	2:B:293:ILE:HD11	1.83	0.60
1:A:420:PRO:HA	1:A:421:PRO:C	2.27	0.60
2:B:79:GLU:O	2:B:82:LYS:HB2	2.02	0.60
1:A:181:CYS:HB3	1:A:188:TYR:HB2	1.84	0.60
2:B:376:THR:O	2:B:380:ILE:HG12	2.02	0.60
2:B:30:LYS:HZ1	2:B:404:GLU:CD	2.10	0.60
2:B:376:THR:CG2	2:B:386:THR:HG22	2.31	0.60
1:A:235:HIS:HB2	1:A:238:LYS:O	2.01	0.59
1:A:332:GLN:HG3	1:A:338:THR:HG23	1.83	0.59
1:A:451:LYS:O	1:A:471:ASP:HA	2.00	0.59
1:A:506:ILE:O	1:A:507:GLN:C	2.45	0.59
1:A:517:LEU:O	1:A:520:GLN:HB2	2.01	0.59
1:A:122:GLU:N	1:A:122:GLU:OE1	2.35	0.59
1:A:295:LEU:HD13	1:A:299:ALA:CB	2.33	0.59
2:B:239:TRP:O	2:B:240:THR:HG23	2.02	0.59
1:A:24:TRP:H	1:A:24:TRP:CD1	2.20	0.59
1:A:312:GLU:O	1:A:312:GLU:HG3	2.02	0.58
1:A:474:ASN:CG	1:A:475:GLN:N	2.60	0.58
2:B:113:ASP:O	2:B:114:ALA:C	2.45	0.58
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.85	0.58
1:A:36:GLU:O	1:A:36:GLU:HG2	2.03	0.58
1:A:130:PHE:O	1:A:143:ARG:HG3	2.03	0.58
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.84	0.58
1:A:246:LEU:C	1:A:307:ARG:NH1	2.62	0.58
1:A:497:THR:O	1:A:535:TRP:HA	2.03	0.58
2:B:356:ARG:HH12	2:B:358:ARG:HA	1.68	0.58
2:B:78:ARG:O	2:B:82:LYS:HG3	2.03	0.58
2:B:266:TRP:NE1	2:B:426:TRP:CD2	2.71	0.58
1:A:495:ILE:O	1:A:533:LEU:HD23	2.04	0.58
1:A:500:GLN:NE2	2:B:422:LEU:HD21	2.19	0.58
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.38	0.58
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.86	0.58
1:A:39:THR:C	1:A:42:GLU:HG2	2.29	0.58
1:A:91:GLN:C	1:A:93:GLY:H	2.12	0.58
1:A:506:ILE:HD12	1:A:506:ILE:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.38	0.58
1:A:317:VAL:HG22	1:A:318:TYR:N	2.18	0.58
2:B:424:LYS:HD3	2:B:425:LEU:N	2.18	0.58
1:A:243:PRO:HG3	1:A:313:PRO:HG2	1.85	0.57
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.85	0.57
1:A:124:PHE:O	1:A:125:ARG:C	2.47	0.57
1:A:361:HIS:CD2	1:A:510:PRO:HB3	2.39	0.57
1:A:451:LYS:CB	1:A:471:ASP:HA	2.33	0.57
2:B:264:LEU:O	2:B:267:ALA:HB3	2.03	0.57
1:A:47:ILE:HD12	1:A:47:ILE:H	1.68	0.57
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.87	0.57
2:B:424:LYS:HD3	2:B:424:LYS:C	2.28	0.57
1:A:27:THR:HG22	1:A:29:GLU:H	1.69	0.57
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.47	0.57
2:B:153:TRP:O	2:B:157:PRO:HD3	2.04	0.57
2:B:168:LEU:O	2:B:172:ARG:HG3	2.05	0.57
1:A:135:ILE:HD12	1:A:135:ILE:N	2.19	0.57
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.87	0.57
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.69	0.57
1:A:480:GLN:HE22	1:A:483:TYR:HD2	1.53	0.57
2:B:191:SER:HB2	2:B:193:LEU:HD23	1.85	0.57
1:A:463:ARG:C	1:A:464:GLN:HG3	2.29	0.56
1:A:77:PHE:O	1:A:80:LEU:N	2.38	0.56
1:A:168:LEU:C	1:A:170:PRO:HD2	2.30	0.56
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.87	0.56
2:B:61:PHE:N	2:B:61:PHE:CD2	2.73	0.56
1:A:253:THR:O	1:A:257:ILE:HG12	2.06	0.56
1:A:500:GLN:CD	2:B:422:LEU:HD11	2.30	0.56
2:B:72:ARG:HH22	2:B:409:THR:HG22	1.71	0.56
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.41	0.56
2:B:257:ILE:HB	2:B:283:LEU:HD11	1.85	0.56
1:A:57:ASN:ND2	1:A:58:THR:H	1.96	0.56
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.41	0.56
1:A:94:ILE:HD12	1:A:94:ILE:N	2.20	0.56
2:B:241:VAL:C	2:B:242:GLN:OE1	2.49	0.56
1:A:42:GLU:HG3	1:A:43:LYS:H	1.71	0.55
1:A:282:LEU:HD22	1:A:282:LEU:N	2.22	0.55
1:A:7:THR:HG22	1:A:119:PRO:O	2.07	0.55
2:B:84:THR:OG1	2:B:154:LYS:HE2	2.06	0.55
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.42	0.55
2:B:60:VAL:HG11	2:B:130:PHE:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:ILE:O	2:B:384:GLY:HA2	2.07	0.55
1:A:358:ARG:HD2	1:A:362:THR:HB	1.87	0.55
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.33	0.55
1:A:17:ASP:O	1:A:83:ARG:HD3	2.07	0.55
1:A:42:GLU:HG3	1:A:43:LYS:N	2.21	0.55
1:A:451:LYS:O	1:A:471:ASP:CA	2.55	0.55
2:B:66:LYS:HG3	2:B:407:GLN:NE2	2.22	0.55
2:B:106:VAL:O	2:B:234:LEU:HB2	2.07	0.55
1:A:132:ILE:O	1:A:142:ILE:HG21	2.07	0.55
1:A:308:GLU:O	1:A:311:LYS:HB2	2.07	0.55
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.42	0.55
1:A:506:ILE:HD12	1:A:506:ILE:N	2.22	0.55
1:A:179:VAL:HG11	3:A:999:FTC:H112	1.87	0.55
1:A:320:ASP:OD2	1:A:322:SER:HB3	2.07	0.55
1:A:356:ARG:NH2	1:A:374:LYS:NZ	2.46	0.55
1:A:517:LEU:HA	1:A:520:GLN:CG	2.35	0.55
1:A:23:GLN:HG2	1:A:131:THR:HG22	1.89	0.55
1:A:130:PHE:O	1:A:131:THR:OG1	2.25	0.55
1:A:306:ASN:O	1:A:310:LEU:HD13	2.06	0.55
1:A:310:LEU:N	1:A:310:LEU:HD12	2.22	0.55
2:B:360:ALA:O	2:B:362:THR:N	2.40	0.55
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.22	0.54
1:A:246:LEU:C	1:A:307:ARG:HH11	2.14	0.54
2:B:33:ALA:O	2:B:37:ILE:HG13	2.06	0.54
2:B:253:THR:O	2:B:257:ILE:HG12	2.08	0.54
2:B:168:LEU:C	2:B:172:ARG:HG3	2.33	0.54
2:B:380:ILE:O	2:B:384:GLY:CA	2.55	0.54
1:A:362:THR:HG23	1:A:366:LYS:CE	2.36	0.54
2:B:358:ARG:HG2	2:B:358:ARG:HH11	1.72	0.54
2:B:205:LEU:HD13	2:B:205:LEU:C	2.33	0.54
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.43	0.54
2:B:120:LEU:HD22	2:B:121:ASP:O	2.08	0.54
1:A:330:GLN:OE1	1:A:340:GLN:OE1	2.25	0.54
1:A:474:ASN:OD1	1:A:475:GLN:HG3	2.08	0.54
1:A:48:SER:O	1:A:49:LYS:HB2	2.07	0.54
1:A:97:PRO:CD	1:A:230:MET:HE2	2.37	0.54
2:B:52:PRO:HD2	2:B:53:GLU:OE2	2.07	0.53
2:B:84:THR:HG22	2:B:124:PHE:HZ	1.73	0.53
2:B:423:VAL:O	2:B:427:TYR:HD2	1.91	0.53
1:A:116:PHE:O	1:A:148:VAL:HG21	2.09	0.53
1:A:120:LEU:CD1	1:A:121:ASP:H	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HG23	1:A:111:VAL:O	2.09	0.53
2:B:132:ILE:HB	2:B:142:ILE:HB	1.90	0.53
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.90	0.53
2:B:39:THR:O	2:B:43:LYS:HG2	2.08	0.53
1:A:416:PHE:CD1	1:A:417:VAL:N	2.76	0.53
1:A:407:GLN:CG	2:B:393:ILE:HA	2.38	0.53
1:A:503:LEU:O	1:A:507:GLN:HB2	2.08	0.53
1:A:546:GLU:HG3	1:A:547:GLN:HE21	1.72	0.53
2:B:371:ALA:O	2:B:372:VAL:C	2.52	0.53
1:A:418:ASN:O	1:A:420:PRO:CD	2.51	0.53
1:A:519:ASN:N	1:A:519:ASN:HD22	2.04	0.53
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.91	0.53
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.89	0.53
1:A:60:VAL:HG11	1:A:73:LYS:NZ	2.24	0.52
2:B:380:ILE:O	2:B:384:GLY:N	2.42	0.52
1:A:92:LEU:C	1:A:92:LEU:HD22	2.35	0.52
1:A:243:PRO:HB3	1:A:313:PRO:HG3	1.92	0.52
1:A:260:LEU:O	1:A:264:LEU:HD23	2.10	0.52
1:A:460:ASN:HA	2:B:286:THR:O	2.10	0.52
1:A:31:ILE:HG21	1:A:134:SER:HA	1.92	0.52
1:A:344:GLU:O	1:A:347:LYS:HB2	2.10	0.52
1:A:499:SER:CB	1:A:502:ALA:HB3	2.34	0.52
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.92	0.52
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.45	0.52
2:B:278:GLN:HA	2:B:278:GLN:HE21	1.74	0.52
1:A:97:PRO:HD2	1:A:230:MET:HE2	1.92	0.52
1:A:295:LEU:HD13	1:A:299:ALA:HB3	1.91	0.52
1:A:46:LYS:CB	1:A:47:ILE:HD12	2.27	0.52
1:A:235:HIS:CD2	1:A:238:LYS:HE3	2.45	0.52
1:A:253:THR:HG23	1:A:256:ASP:OD1	2.09	0.52
2:B:66:LYS:HG3	2:B:407:GLN:CD	2.35	0.52
1:A:324:ASP:O	1:A:343:GLN:HG2	2.10	0.52
1:A:536:VAL:HG23	1:A:542:ILE:HD13	1.91	0.52
1:A:241:VAL:O	1:A:243:PRO:N	2.43	0.52
2:B:85:GLN:O	2:B:85:GLN:HG3	2.08	0.52
1:A:522:ILE:O	1:A:526:ILE:HG13	2.09	0.52
2:B:53:GLU:CD	2:B:53:GLU:H	2.18	0.52
1:A:193:LEU:HB3	1:A:197:GLN:HB3	1.92	0.51
1:A:358:ARG:NH2	1:A:513:SER:CA	2.72	0.51
1:A:358:ARG:HD2	1:A:362:THR:CB	2.40	0.51
2:B:325:LEU:HD12	2:B:343:GLN:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:SER:HB2	1:A:493:VAL:HG21	1.92	0.51
1:A:516:GLU:O	1:A:519:ASN:HB2	2.09	0.51
1:A:516:GLU:O	1:A:520:GLN:HG2	2.10	0.51
2:B:199:ARG:O	2:B:203:GLU:HB2	2.10	0.51
1:A:7:THR:HG21	1:A:120:LEU:O	2.11	0.51
2:B:193:LEU:N	2:B:193:LEU:HD22	2.26	0.51
1:A:47:ILE:HG21	1:A:144:TYR:CD2	2.46	0.51
1:A:474:ASN:CG	1:A:475:GLN:H	2.18	0.51
2:B:389:PHE:HB3	2:B:391:LEU:CD2	2.40	0.51
1:A:126:LYS:C	1:A:128:THR:H	2.18	0.51
2:B:264:LEU:O	2:B:267:ALA:N	2.44	0.51
1:A:296:THR:CG2	1:A:298:GLU:OE2	2.57	0.51
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.46	0.51
2:B:175:ASN:HD21	2:B:201:LYS:HZ3	1.53	0.51
1:A:274:ILE:CD1	1:A:310:LEU:HD11	2.29	0.51
1:A:282:LEU:O	1:A:293:ILE:HD13	2.11	0.50
1:A:344:GLU:HB2	1:A:347:LYS:HB2	1.93	0.50
1:A:439:THR:O	1:A:459:THR:HA	2.10	0.50
1:A:523:GLU:HB3	1:A:527:LYS:HZ3	1.76	0.50
2:B:266:TRP:CD1	2:B:266:TRP:C	2.89	0.50
1:A:345:PRO:O	1:A:346:PHE:HB2	2.11	0.50
1:A:356:ARG:HH22	1:A:374:LYS:HE3	1.77	0.50
1:A:447:ASN:CB	1:A:450:THR:HG23	2.36	0.50
1:A:60:VAL:CG1	1:A:73:LYS:NZ	2.75	0.50
1:A:296:THR:O	1:A:299:ALA:HB3	2.12	0.50
2:B:276:VAL:HG22	2:B:276:VAL:O	2.11	0.50
2:B:406:TRP:HZ2	2:B:410:TRP:O	1.95	0.50
1:A:17:ASP:OD2	1:A:18:GLY:N	2.44	0.50
1:A:451:LYS:HB2	1:A:471:ASP:HA	1.94	0.50
1:A:508:ALA:O	1:A:509:GLN:C	2.55	0.50
2:B:7:THR:HG23	2:B:7:THR:O	2.12	0.50
2:B:100:LEU:N	2:B:100:LEU:HD23	2.27	0.50
1:A:543:GLY:HA2	1:A:546:GLU:HG2	1.93	0.50
2:B:332:GLN:OE1	2:B:424:LYS:HE3	2.12	0.50
1:A:194:GLU:HG2	1:A:195:ILE:N	2.26	0.50
2:B:368:LEU:O	2:B:372:VAL:HG23	2.11	0.50
1:A:24:TRP:H	1:A:24:TRP:HD1	1.59	0.50
1:A:90:VAL:O	1:A:91:GLN:CB	2.59	0.50
2:B:193:LEU:HD22	2:B:193:LEU:H	1.77	0.50
1:A:309:ILE:C	1:A:311:LYS:H	2.20	0.49
1:A:356:ARG:HG2	1:A:357:MET:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:CG1	1:A:419:THR:HG22	2.35	0.49
2:B:171:PHE:CG	2:B:205:LEU:HD23	2.47	0.49
2:B:345:PRO:O	2:B:346:PHE:HB2	2.12	0.49
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.47	0.49
1:A:122:GLU:CD	1:A:122:GLU:N	2.70	0.49
2:B:326:ILE:HB	2:B:342:TYR:O	2.11	0.49
2:B:423:VAL:O	2:B:427:TYR:CD2	2.66	0.49
1:A:114:ALA:CB	1:A:160:PHE:CE2	2.95	0.49
1:A:500:GLN:HE22	2:B:422:LEU:CD1	2.24	0.49
1:A:34:LEU:HA	1:A:37:ILE:HG22	1.94	0.49
1:A:111:VAL:O	1:A:114:ALA:HB2	2.13	0.49
2:B:100:LEU:HD23	2:B:101:LYS:H	1.78	0.49
1:A:54:ASN:HD22	1:A:126:LYS:HB3	1.78	0.49
1:A:513:SER:HB3	1:A:519:ASN:HD21	1.76	0.49
1:A:63:ILE:HD12	1:A:64:LYS:H	1.78	0.49
1:A:210:LEU:HD12	1:A:215:THR:HA	1.91	0.49
2:B:51:GLY:HA3	2:B:53:GLU:OE2	2.12	0.49
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.13	0.48
2:B:118:VAL:HG13	2:B:119:PRO:HD2	1.95	0.48
2:B:296:THR:CG2	2:B:298:GLU:OE1	2.60	0.48
1:A:173:LYS:O	1:A:173:LYS:HD3	2.13	0.48
1:A:356:ARG:NH1	1:A:374:LYS:NZ	2.61	0.48
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.81	0.48
2:B:426:TRP:O	2:B:429:LEU:HB2	2.13	0.48
1:A:126:LYS:O	1:A:128:THR:N	2.46	0.48
1:A:282:LEU:H	1:A:282:LEU:CD2	2.26	0.48
2:B:61:PHE:CE1	2:B:403:THR:HG22	2.47	0.48
2:B:175:ASN:ND2	2:B:201:LYS:HZ1	2.04	0.48
2:B:296:THR:CG2	2:B:298:GLU:HB2	2.43	0.48
1:A:46:LYS:HE3	1:A:116:PHE:CG	2.46	0.48
1:A:247:PRO:C	1:A:307:ARG:HH12	2.22	0.48
1:A:390:LYS:HE2	1:A:415:GLU:CD	2.39	0.48
2:B:60:VAL:HG11	2:B:130:PHE:HD1	1.76	0.48
1:A:49:LYS:HA	1:A:144:TYR:HA	1.96	0.48
1:A:113:ASP:O	1:A:113:ASP:OD1	2.32	0.48
1:A:301:LEU:HD23	1:A:301:LEU:O	2.14	0.48
1:A:502:ALA:O	1:A:506:ILE:HD13	2.12	0.48
2:B:183:TYR:O	2:B:186:ASP:HB2	2.14	0.48
2:B:240:THR:O	2:B:350:LYS:HG3	2.12	0.48
1:A:92:LEU:HD21	2:B:137:ASN:OD1	2.13	0.48
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ILE:HG22	1:A:330:GLN:N	2.28	0.48
1:A:376:THR:HG23	1:A:386:THR:HB	1.95	0.48
1:A:246:LEU:HB2	1:A:307:ARG:HH11	1.78	0.48
1:A:293:ILE:HG22	1:A:294:PRO:O	2.14	0.48
1:A:396:GLU:O	1:A:400:THR:HG23	2.14	0.48
1:A:517:LEU:HA	1:A:520:GLN:HG3	1.95	0.48
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.28	0.48
1:A:34:LEU:HD21	1:A:62:ALA:CB	2.35	0.48
1:A:345:PRO:C	1:A:346:PHE:HD1	2.21	0.48
1:A:447:ASN:HD22	1:A:448:ARG:N	2.11	0.48
2:B:154:LYS:O	2:B:157:PRO:HD2	2.13	0.48
1:A:111:VAL:HG22	1:A:185:ASP:O	2.13	0.48
1:A:279:LEU:O	1:A:280:CSD:C	2.62	0.48
1:A:258:GLN:HE22	1:A:289:LEU:CD1	2.26	0.48
1:A:465:LYS:O	1:A:466:VAL:HG23	2.14	0.48
1:A:500:GLN:HE22	2:B:422:LEU:CD2	2.26	0.48
1:A:77:PHE:O	1:A:78:ARG:C	2.57	0.47
1:A:394:GLN:HG2	1:A:396:GLU:OE2	2.13	0.47
1:A:447:ASN:HD22	1:A:447:ASN:C	2.20	0.47
2:B:28:GLU:O	2:B:31:ILE:N	2.47	0.47
2:B:63:ILE:HD13	2:B:63:ILE:H	1.78	0.47
2:B:370:GLU:O	2:B:373:GLN:HB2	2.14	0.47
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.44	0.47
1:A:358:ARG:HH22	1:A:514:GLU:CA	2.24	0.47
2:B:264:LEU:O	2:B:265:ASN:C	2.57	0.47
1:A:34:LEU:CD2	1:A:73:LYS:HA	2.44	0.47
1:A:46:LYS:O	1:A:147:ASN:ND2	2.46	0.47
2:B:254:VAL:HG21	2:B:287:LYS:HB2	1.96	0.47
1:A:2:ILE:HD11	1:A:45:GLY:CA	2.42	0.47
1:A:37:ILE:HD13	1:A:73:LYS:N	2.30	0.47
1:A:235:HIS:CG	1:A:238:LYS:HE3	2.49	0.47
1:A:536:VAL:CG2	1:A:542:ILE:HD13	2.44	0.47
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.97	0.47
1:A:125:ARG:O	1:A:126:LYS:C	2.57	0.47
1:A:411:ILE:HG22	1:A:412:PRO:O	2.14	0.47
2:B:100:LEU:HA	2:B:103:LYS:HB2	1.96	0.47
2:B:277:ARG:HA	2:B:277:ARG:NE	2.28	0.47
1:A:46:LYS:CE	1:A:116:PHE:CD2	2.90	0.47
1:A:77:PHE:O	1:A:79:GLU:N	2.47	0.47
2:B:209:LEU:C	2:B:211:ARG:N	2.71	0.47
2:B:278:GLN:HE21	2:B:278:GLN:CA	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:O	1:A:56:TYR:HA	2.14	0.47
1:A:34:LEU:HD22	1:A:73:LYS:HG2	1.96	0.47
1:A:47:ILE:HG22	1:A:48:SER:O	2.14	0.47
2:B:171:PHE:CD2	2:B:205:LEU:HD23	2.50	0.47
1:A:66:LYS:HD2	1:A:66:LYS:N	2.27	0.47
1:A:124:PHE:O	1:A:127:TYR:N	2.48	0.47
1:A:124:PHE:C	1:A:126:LYS:N	2.72	0.47
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.49	0.47
1:A:356:ARG:HB2	1:A:356:ARG:CZ	2.45	0.47
1:A:457:TYR:CE2	1:A:465:LYS:HD2	2.43	0.47
1:A:484:LEU:HD23	1:A:487:GLN:OE1	2.14	0.47
1:A:91:GLN:C	1:A:93:GLY:N	2.73	0.47
1:A:122:GLU:HA	1:A:125:ARG:NE	2.30	0.47
2:B:296:THR:HB	2:B:299:ALA:H	1.79	0.47
1:A:40:GLU:O	1:A:41:MET:C	2.58	0.46
1:A:244:ILE:HG12	1:A:245:VAL:N	2.29	0.46
2:B:259:LYS:O	2:B:260:LEU:C	2.58	0.46
1:A:203:GLU:O	1:A:204:GLU:C	2.56	0.46
1:A:234:LEU:HD12	3:A:999:FTC:HB1	1.96	0.46
1:A:257:ILE:O	1:A:261:VAL:HG23	2.14	0.46
1:A:463:ARG:O	1:A:464:GLN:HG3	2.15	0.46
1:A:481:ALA:O	1:A:484:LEU:HB2	2.14	0.46
2:B:72:ARG:HH21	2:B:151:GLN:NE2	2.13	0.46
1:A:252:TRP:HB3	1:A:257:ILE:HD11	1.97	0.46
1:A:499:SER:HB2	1:A:502:ALA:CB	2.35	0.46
2:B:278:GLN:HB3	2:B:299:ALA:HA	1.95	0.46
1:A:109:LEU:HD12	1:A:109:LEU:H	1.78	0.46
2:B:120:LEU:HD23	2:B:121:ASP:H	1.78	0.46
1:A:486:LEU:CB	1:A:524:GLN:HG2	2.43	0.46
1:A:493:VAL:HG12	1:A:494:ASN:N	2.31	0.46
1:A:358:ARG:NH2	1:A:514:GLU:H	2.08	0.46
1:A:382:ILE:HG22	1:A:383:TRP:CE2	2.50	0.46
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.44	0.46
2:B:158:ALA:O	2:B:161:GLN:HB2	2.16	0.46
1:A:229:TRP:C	1:A:231:GLY:H	2.23	0.46
1:A:295:LEU:HD13	1:A:299:ALA:HB1	1.97	0.46
1:A:447:ASN:O	1:A:450:THR:O	2.33	0.46
2:B:160:PHE:O	2:B:161:GLN:C	2.59	0.46
2:B:185:ASP:OD2	2:B:185:ASP:N	2.49	0.46
1:A:218:ASP:O	1:A:221:HIS:N	2.39	0.46
1:A:253:THR:O	1:A:256:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:O	1:A:242:GLN:C	2.60	0.45
1:A:438:GLU:CG	1:A:461:ARG:HD2	2.46	0.45
1:A:34:LEU:HA	1:A:37:ILE:CG2	2.45	0.45
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.68	0.45
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.51	0.45
1:A:477:THR:O	1:A:478:GLU:C	2.59	0.45
2:B:198:HIS:O	2:B:201:LYS:N	2.49	0.45
1:A:447:ASN:O	1:A:448:ARG:C	2.59	0.45
2:B:175:ASN:C	2:B:177:ASP:H	2.24	0.45
1:A:27:THR:HG22	1:A:28:GLU:N	2.31	0.45
1:A:44:GLU:HB3	1:A:45:GLY:H	1.48	0.45
1:A:191:SER:OG	1:A:198:HIS:ND1	2.43	0.45
1:A:329:ILE:O	1:A:392:PRO:HD3	2.17	0.45
1:A:359:GLY:C	1:A:361:HIS:H	2.24	0.45
1:A:506:ILE:H	1:A:506:ILE:CD1	2.28	0.45
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.97	0.45
2:B:201:LYS:HD2	2:B:201:LYS:HA	1.77	0.45
2:B:374:LYS:O	2:B:378:GLU:HG3	2.17	0.45
1:A:358:ARG:CZ	1:A:513:SER:C	2.89	0.45
1:A:361:HIS:NE2	1:A:508:ALA:HB1	2.31	0.45
2:B:395:LYS:HG2	2:B:399:GLU:OE2	2.17	0.45
1:A:241:VAL:CG2	1:A:270:ILE:HD13	2.45	0.45
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.16	0.45
2:B:121:ASP:O	2:B:125:ARG:HG3	2.17	0.45
2:B:175:ASN:ND2	2:B:201:LYS:HZ3	2.12	0.45
2:B:374:LYS:O	2:B:377:THR:HB	2.15	0.45
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.45	0.45
1:A:79:GLU:O	1:A:80:LEU:C	2.60	0.45
1:A:248:GLU:OE2	1:A:307:ARG:NH2	2.50	0.45
1:A:456:GLY:HA3	1:A:466:VAL:HG22	1.97	0.45
2:B:63:ILE:O	2:B:72:ARG:HB3	2.17	0.45
1:A:358:ARG:HD2	1:A:362:THR:OG1	2.16	0.45
2:B:53:GLU:O	2:B:55:PRO:HD3	2.16	0.45
2:B:162:SER:OG	2:B:163:SER:N	2.50	0.45
2:B:195:ILE:HA	2:B:198:HIS:HB3	1.99	0.45
1:A:47:ILE:CD1	1:A:47:ILE:N	2.77	0.45
1:A:169:GLU:N	1:A:170:PRO:HD2	2.31	0.45
1:A:376:THR:O	1:A:380:ILE:HD12	2.17	0.45
1:A:489:SER:CB	1:A:493:VAL:HG21	2.47	0.45
2:B:317:VAL:HG23	2:B:317:VAL:O	2.16	0.45
1:A:40:GLU:O	1:A:42:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HG22	1:A:48:SER:C	2.42	0.45
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.73	0.45
1:A:356:ARG:CZ	1:A:356:ARG:CB	2.94	0.45
2:B:184:MET:C	2:B:186:ASP:H	2.25	0.45
2:B:115:TYR:HE1	2:B:157:PRO:HA	1.81	0.44
1:A:96:HIS:NE2	1:A:350:LYS:HE2	2.32	0.44
1:A:228:LEU:CD2	1:A:228:LEU:N	2.60	0.44
1:A:332:GLN:HG3	1:A:338:THR:HG21	1.98	0.44
2:B:168:LEU:O	2:B:169:GLU:C	2.60	0.44
1:A:480:GLN:O	1:A:481:ALA:C	2.59	0.44
2:B:106:VAL:HG22	2:B:190:GLY:HA3	2.00	0.44
2:B:278:GLN:HB2	2:B:302:GLU:CD	2.43	0.44
1:A:2:ILE:HG22	1:A:3:SER:N	2.33	0.44
1:A:23:GLN:OE1	1:A:133:PRO:HG3	2.17	0.44
1:A:184:MET:HB3	1:A:185:ASP:H	1.41	0.44
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.99	0.44
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.99	0.44
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.47	0.44
2:B:255:ASN:O	2:B:256:ASP:C	2.61	0.44
1:A:111:VAL:O	1:A:112:GLY:C	2.59	0.44
1:A:129:ALA:HA	1:A:144:TYR:O	2.18	0.44
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.53	0.44
1:A:405:TYR:HE2	1:A:407:GLN:HB3	1.80	0.44
1:A:472:THR:OG1	1:A:473:THR:N	2.50	0.44
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.99	0.44
2:B:398:TRP:O	2:B:402:TRP:HD1	2.01	0.44
1:A:46:LYS:HB3	1:A:47:ILE:CD1	2.29	0.44
1:A:311:LYS:O	1:A:313:PRO:HD3	2.18	0.44
1:A:477:THR:O	1:A:480:GLN:HB3	2.16	0.44
2:B:13:LYS:HG2	2:B:85:GLN:HA	1.99	0.44
2:B:208:HIS:O	2:B:211:ARG:HB3	2.18	0.44
1:A:97:PRO:HD3	1:A:230:MET:HE2	2.00	0.44
1:A:130:PHE:HB2	1:A:144:TYR:N	2.20	0.44
2:B:296:THR:HG21	2:B:298:GLU:HB2	2.00	0.44
1:A:366:LYS:HB3	1:A:366:LYS:HE2	1.81	0.44
1:A:412:PRO:O	1:A:413:GLU:C	2.61	0.44
1:A:452:LEU:HD12	1:A:469:LEU:O	2.18	0.44
1:A:543:GLY:O	1:A:545:ASN:N	2.48	0.44
1:A:124:PHE:O	1:A:126:LYS:N	2.51	0.44
1:A:60:VAL:CG1	1:A:73:LYS:HZ1	2.29	0.43
1:A:125:ARG:O	1:A:128:THR:OG1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLN:HA	1:A:182:GLN:HE22	1.83	0.43
1:A:170:PRO:CG	1:A:171:PHE:H	2.27	0.43
1:A:287:LYS:HG3	1:A:288:ALA:N	2.33	0.43
1:A:451:LYS:HA	1:A:472:THR:O	2.18	0.43
2:B:28:GLU:O	2:B:29:GLU:C	2.61	0.43
2:B:167:ILE:O	2:B:208:HIS:NE2	2.40	0.43
2:B:360:ALA:C	2:B:362:THR:N	2.76	0.43
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.53	0.43
2:B:399:GLU:HA	2:B:402:TRP:HD1	1.83	0.43
1:A:114:ALA:O	1:A:118:VAL:HG23	2.17	0.43
1:A:218:ASP:O	1:A:222:GLN:HG3	2.18	0.43
1:A:243:PRO:CG	1:A:313:PRO:HG2	2.48	0.43
1:A:254:VAL:O	1:A:255:ASN:C	2.62	0.43
1:A:310:LEU:N	1:A:310:LEU:CD1	2.81	0.43
1:A:515:SER:CB	1:A:518:VAL:HG23	2.48	0.43
1:A:517:LEU:HA	1:A:520:GLN:HG2	1.98	0.43
2:B:358:ARG:HG2	2:B:358:ARG:NH1	2.33	0.43
1:A:58:THR:HG22	1:A:76:ASP:O	2.19	0.43
1:A:210:LEU:HD12	1:A:210:LEU:HA	1.91	0.43
1:A:358:ARG:CZ	1:A:513:SER:CA	2.95	0.43
1:A:419:THR:HG23	1:A:419:THR:O	2.19	0.43
1:A:460:ASN:HD21	1:A:461:ARG:HH11	1.66	0.43
2:B:360:ALA:C	2:B:362:THR:H	2.27	0.43
1:A:237:ASP:OD2	1:A:237:ASP:N	2.51	0.43
1:A:507:GLN:C	1:A:509:GLN:H	2.26	0.43
2:B:180:ILE:HG12	2:B:189:VAL:HG13	2.00	0.43
1:A:64:LYS:HB2	1:A:66:LYS:NZ	2.34	0.43
1:A:77:PHE:HD2	1:A:80:LEU:CD2	2.31	0.43
2:B:263:LYS:O	2:B:266:TRP:HD1	2.02	0.43
2:B:378:GLU:O	2:B:379:SER:C	2.59	0.43
1:A:201:LYS:HD3	1:A:204:GLU:OE1	2.19	0.43
2:B:76:ASP:OD2	2:B:76:ASP:C	2.60	0.43
2:B:120:LEU:CD2	2:B:121:ASP:N	2.81	0.43
1:A:118:VAL:CG1	1:A:119:PRO:HD2	2.49	0.43
1:A:229:TRP:CG	1:A:230:MET:H	2.36	0.43
1:A:255:ASN:HB2	1:A:289:LEU:HG	2.01	0.43
1:A:361:HIS:HE2	1:A:508:ALA:HB1	1.83	0.43
2:B:100:LEU:N	2:B:100:LEU:CD2	2.82	0.43
2:B:211:ARG:HG3	2:B:211:ARG:HH11	1.83	0.43
2:B:161:GLN:O	2:B:162:SER:C	2.62	0.43
2:B:165:THR:OG1	2:B:166:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:ALA:C	2:B:269:GLN:N	2.77	0.43
1:A:23:GLN:C	1:A:23:GLN:CD	2.87	0.42
1:A:85:GLN:HG3	1:A:86:ASP:N	2.33	0.42
2:B:84:THR:HG22	2:B:124:PHE:CZ	2.54	0.42
2:B:206:ARG:NH1	2:B:206:ARG:HG2	2.34	0.42
2:B:366:LYS:HG2	2:B:370:GLU:OE2	2.18	0.42
2:B:184:MET:HB3	2:B:185:ASP:H	1.65	0.42
2:B:188:TYR:CE1	2:B:380:ILE:HG21	2.54	0.42
2:B:401:TRP:HB3	2:B:405:TYR:HE1	1.84	0.42
1:A:104:LYS:HD2	1:A:192:ASP:C	2.44	0.42
1:A:301:LEU:HD23	1:A:301:LEU:C	2.44	0.42
1:A:332:GLN:HE21	1:A:332:GLN:HB3	1.47	0.42
2:B:193:LEU:H	2:B:193:LEU:CD2	2.32	0.42
2:B:267:ALA:O	2:B:269:GLN:N	2.51	0.42
2:B:314:VAL:HG22	2:B:315:HIS:N	2.34	0.42
1:A:41:MET:CB	1:A:47:ILE:CD1	2.76	0.42
1:A:362:THR:HG23	1:A:366:LYS:HE3	2.02	0.42
1:A:493:VAL:CG1	1:A:494:ASN:N	2.83	0.42
2:B:57:ASN:HD21	2:B:131:THR:N	2.18	0.42
2:B:72:ARG:NH2	2:B:409:THR:HG22	2.34	0.42
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.50	0.42
1:A:505:ILE:O	1:A:510:PRO:HD3	2.20	0.42
1:A:91:GLN:O	1:A:93:GLY:N	2.52	0.42
1:A:516:GLU:CG	1:A:517:LEU:N	2.79	0.42
2:B:120:LEU:HD21	2:B:124:PHE:HB3	2.00	0.42
1:A:129:ALA:HB1	1:A:143:ARG:NH2	2.34	0.42
1:A:260:LEU:HD23	1:A:279:LEU:HD13	2.01	0.42
1:A:358:ARG:HD2	1:A:512:GLN:HG3	2.01	0.42
2:B:77:PHE:O	2:B:78:ARG:C	2.61	0.42
2:B:353:LYS:HG2	2:B:354:TYR:N	2.34	0.42
1:A:34:LEU:O	1:A:37:ILE:HG22	2.20	0.42
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.20	0.42
1:A:423:VAL:O	1:A:423:VAL:CG2	2.65	0.42
1:A:438:GLU:HG2	1:A:459:THR:HB	2.00	0.42
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.60	0.42
2:B:116:PHE:CE2	2:B:151:GLN:OE1	2.73	0.42
1:A:243:PRO:CG	1:A:313:PRO:CG	2.95	0.42
1:A:320:ASP:CG	1:A:323:LYS:HG2	2.45	0.42
1:A:122:GLU:HA	1:A:125:ARG:HE	1.83	0.42
1:A:296:THR:HB	1:A:299:ALA:H	1.83	0.42
1:A:356:ARG:NH1	1:A:374:LYS:HZ3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:HD12	1:A:491:LEU:N	2.34	0.42
1:A:295:LEU:O	1:A:296:THR:C	2.61	0.41
1:A:402:TRP:HB2	1:A:409:THR:CG2	2.50	0.41
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.50	0.41
1:A:492:GLU:HA	1:A:530:LYS:O	2.20	0.41
2:B:171:PHE:HZ	2:B:201:LYS:HG3	1.85	0.41
1:A:118:VAL:O	1:A:149:LEU:HD13	2.19	0.41
1:A:170:PRO:HG2	1:A:171:PHE:N	2.28	0.41
1:A:179:VAL:CG1	3:A:999:FTC:H112	2.49	0.41
1:A:210:LEU:C	1:A:212:TRP:N	2.70	0.41
1:A:122:GLU:C	1:A:124:PHE:H	2.28	0.41
1:A:419:THR:O	1:A:420:PRO:C	2.63	0.41
1:A:38:CYS:HB3	1:A:144:TYR:CZ	2.56	0.41
1:A:325:LEU:HD22	1:A:341:ILE:CG2	2.51	0.41
1:A:376:THR:HG22	1:A:380:ILE:CD1	2.50	0.41
2:B:333:GLY:O	2:B:334:GLN:C	2.63	0.41
1:A:130:PHE:O	1:A:143:ARG:NH1	2.53	0.41
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.50	0.41
1:A:358:ARG:NH2	1:A:359:GLY:O	2.48	0.41
1:A:396:GLU:H	1:A:396:GLU:CD	2.27	0.41
2:B:120:LEU:O	2:B:121:ASP:C	2.63	0.41
2:B:185:ASP:HB2	2:B:409:THR:HG21	2.02	0.41
2:B:422:LEU:HD12	2:B:422:LEU:N	2.33	0.41
1:A:358:ARG:HD3	1:A:512:GLN:HE21	1.85	0.41
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.20	0.41
1:A:18:GLY:HA2	1:A:19:PRO:HD3	1.94	0.41
1:A:40:GLU:C	1:A:42:GLU:N	2.77	0.41
1:A:77:PHE:HD2	1:A:80:LEU:HD23	1.84	0.41
1:A:410:TRP:CG	1:A:411:ILE:N	2.89	0.41
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.35	0.41
1:A:41:MET:SD	1:A:47:ILE:HD11	2.60	0.41
1:A:94:ILE:N	1:A:94:ILE:CD1	2.83	0.41
1:A:96:HIS:HD2	1:A:230:MET:HE1	1.82	0.41
1:A:199:ARG:O	1:A:202:ILE:HB	2.20	0.41
1:A:279:LEU:CA	1:A:282:LEU:HD23	2.43	0.41
1:A:362:THR:CG2	1:A:363:ASN:N	2.80	0.41
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.56	0.41
2:B:164:MET:O	2:B:167:ILE:HB	2.21	0.41
2:B:169:GLU:C	2:B:171:PHE:H	2.29	0.41
2:B:383:TRP:O	2:B:384:GLY:C	2.64	0.41
2:B:392:PRO:HG2	2:B:392:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:C	1:A:37:ILE:HG22	2.46	0.41
1:A:210:LEU:HD11	1:A:215:THR:HB	2.02	0.41
1:A:465:LYS:C	1:A:466:VAL:HG23	2.46	0.41
2:B:118:VAL:CG1	2:B:119:PRO:HD2	2.51	0.41
2:B:139:THR:HG22	2:B:140:PRO:CD	2.50	0.41
1:A:242:GLN:O	1:A:243:PRO:C	2.65	0.40
1:A:246:LEU:H	1:A:246:LEU:HG	1.54	0.40
1:A:320:ASP:OD1	1:A:323:LYS:HG2	2.21	0.40
2:B:13:LYS:HG3	2:B:83:ARG:O	2.21	0.40
2:B:66:LYS:HE2	2:B:66:LYS:HB2	1.89	0.40
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.37	0.40
1:A:173:LYS:C	1:A:173:LYS:CD	2.94	0.40
1:A:258:GLN:NE2	1:A:289:LEU:HD11	2.33	0.40
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.57	0.40
1:A:205:LEU:O	1:A:205:LEU:HD12	2.22	0.40
1:A:241:VAL:CG2	1:A:314:VAL:HB	2.52	0.40
1:A:243:PRO:HG3	1:A:313:PRO:CB	2.50	0.40
1:A:447:ASN:C	1:A:447:ASN:ND2	2.79	0.40
2:B:109:LEU:N	2:B:187:LEU:O	2.44	0.40
2:B:298:GLU:CD	2:B:298:GLU:N	2.79	0.40
1:A:305:GLU:O	1:A:309:ILE:HG12	2.22	0.40
2:B:121:ASP:C	2:B:121:ASP:OD1	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	528/560 (94%)	409 (78%)	89 (17%)	30 (6%)	1	8
2	B	396/440 (90%)	336 (85%)	49 (12%)	11 (3%)	4	21
All	All	924/1000 (92%)	745 (81%)	138 (15%)	41 (4%)	2	12

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	112	GLY
1	A	127	TYR
1	A	195	ILE
2	B	356	ARG
2	B	361	HIS
1	A	44	GLU
1	A	78	ARG
1	A	89	GLU
1	A	92	LEU
1	A	360	ALA
1	A	505	ILE
1	A	508	ALA
2	B	268	SER
2	B	358	ARG
2	B	382	ILE
1	A	41	MET
1	A	49	LYS
1	A	52	PRO
1	A	131	THR
1	A	451	LYS
1	A	85	GLN
1	A	310	LEU
1	A	313	PRO
1	A	420	PRO
1	A	487	GLN
2	B	162	SER
1	A	19	PRO
1	A	419	THR
1	A	489	SER
1	A	543	GLY
2	B	240	THR
2	B	310	LEU
2	B	371	ALA
2	B	423	VAL
1	A	25	PRO
1	A	157	PRO
1	A	311	LYS
2	B	170	PRO
1	A	542	ILE
1	A	276	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	477/499 (96%)	424 (89%)	53 (11%)	6	25
2	B	366/400 (92%)	342 (93%)	24 (7%)	15	46
All	All	843/899 (94%)	766 (91%)	77 (9%)	9	33

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	23	GLN
1	A	24	TRP
1	A	29	GLU
1	A	36	GLU
1	A	44	GLU
1	A	46	LYS
1	A	47	ILE
1	A	63	ILE
1	A	89	GLU
1	A	92	LEU
1	A	107	THR
1	A	108	VAL
1	A	109	LEU
1	A	122	GLU
1	A	151	GLN
1	A	173	LYS
1	A	184	MET
1	A	187	LEU
1	A	194	GLU
1	A	197	GLN
1	A	215	THR
1	A	216	THR
1	A	240	THR
1	A	246	LEU
1	A	253	THR
1	A	274	ILE

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Mol	Chain	Res	Type
1	A	295	LEU
1	A	296	THR
1	A	330	GLN
1	A	332	GLN
1	A	336	GLN
1	A	340	GLN
1	A	357	MET
1	A	358	ARG
1	A	368	LEU
1	A	373	GLN
1	A	377	THR
1	A	386	THR
1	A	394	GLN
1	A	417	VAL
1	A	418	ASN
1	A	423	VAL
1	A	432	GLU
1	A	450	THR
1	A	458	VAL
1	A	459	THR
1	A	488	ASP
1	A	496	VAL
1	A	533	LEU
1	A	536	VAL
1	A	537	PRO
1	A	545	ASN
2	B	24	TRP
2	B	53	GLU
2	B	60	VAL
2	B	61	PHE
2	B	63	ILE
2	B	120	LEU
2	B	161	GLN
2	B	185	ASP
2	B	203	GLU
2	B	205	LEU
2	B	242	GLN
2	B	247	PRO
2	B	250	ASP
2	B	266	TRP
2	B	283	LEU
2	B	303	LEU

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Mol	Chain	Res	Type
2	B	336	GLN
2	B	353	LYS
2	B	358	ARG
2	B	368	LEU
2	B	379	SER
2	B	422	LEU
2	B	425	LEU
2	B	431	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	145	GLN
1	A	182	GLN
1	A	197	GLN
1	A	207	GLN
1	A	222	GLN
1	A	235	HIS
1	A	255	ASN
1	A	258	GLN
1	A	278	GLN
1	A	332	GLN
1	A	334	GLN
1	A	340	GLN
1	A	394	GLN
1	A	418	ASN
1	A	428	GLN
1	A	447	ASN
1	A	475	GLN
1	A	480	GLN
1	A	507	GLN
1	A	512	GLN
1	A	519	ASN
1	A	524	GLN
1	A	545	ASN
1	A	547	GLN
2	B	57	ASN
2	B	96	HIS
2	B	145	GLN
2	B	151	GLN

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Mol	Chain	Res	Type
2	B	174	GLN
2	B	175	ASN
2	B	235	HIS
2	B	255	ASN
2	B	269	GLN
2	B	278	GLN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSD	A	280	1	4,7,8	1.40	0	1,8,10	8.65	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	8.65	121.53	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
3	FTC	A	999	-	24,24,24	1.77	6 (25%)	29,31,31	2.09	11 (37%)

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
3	FTC	A	999	-	-	6/13/13/13	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FTC	C13-N14	4.07	1.39	1.34
3	A	999	FTC	C1-N2	3.16	1.39	1.34
3	A	999	FTC	C9-S9	2.50	1.73	1.68
3	A	999	FTC	C3-N2	2.48	1.39	1.34
3	A	999	FTC	C17-C18	2.21	1.42	1.39
3	A	999	FTC	C15-N14	2.04	1.38	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	FTC	C3-N2-C1	4.96	122.49	117.83
3	A	999	FTC	C15-N14-C13	4.63	123.67	117.79
3	A	999	FTC	C16-C15-N14	-4.23	118.78	123.97
3	A	999	FTC	N8-C1-N2	2.54	122.49	114.87
3	A	999	FTC	C6-C1-N2	-2.46	118.86	122.61
3	A	999	FTC	C1-N8-C9	2.33	133.25	130.74
3	A	999	FTC	N8-C9-N10	2.25	119.40	114.19
3	A	999	FTC	S9-C9-N8	-2.23	117.87	124.33
3	A	999	FTC	C6-C5-C4	2.17	121.42	119.24
3	A	999	FTC	O17-C17-C18	2.16	119.18	115.92
3	A	999	FTC	C4-C3-N2	-2.13	119.53	122.26

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	FTC	N8-C9-N10-C11
3	A	999	FTC	S9-C9-N10-C11
3	A	999	FTC	C18-C17-O17-CA
3	A	999	FTC	N10-C11-C12-C13
3	A	999	FTC	CB-CA-O17-C17
3	A	999	FTC	C16-C17-O17-CA

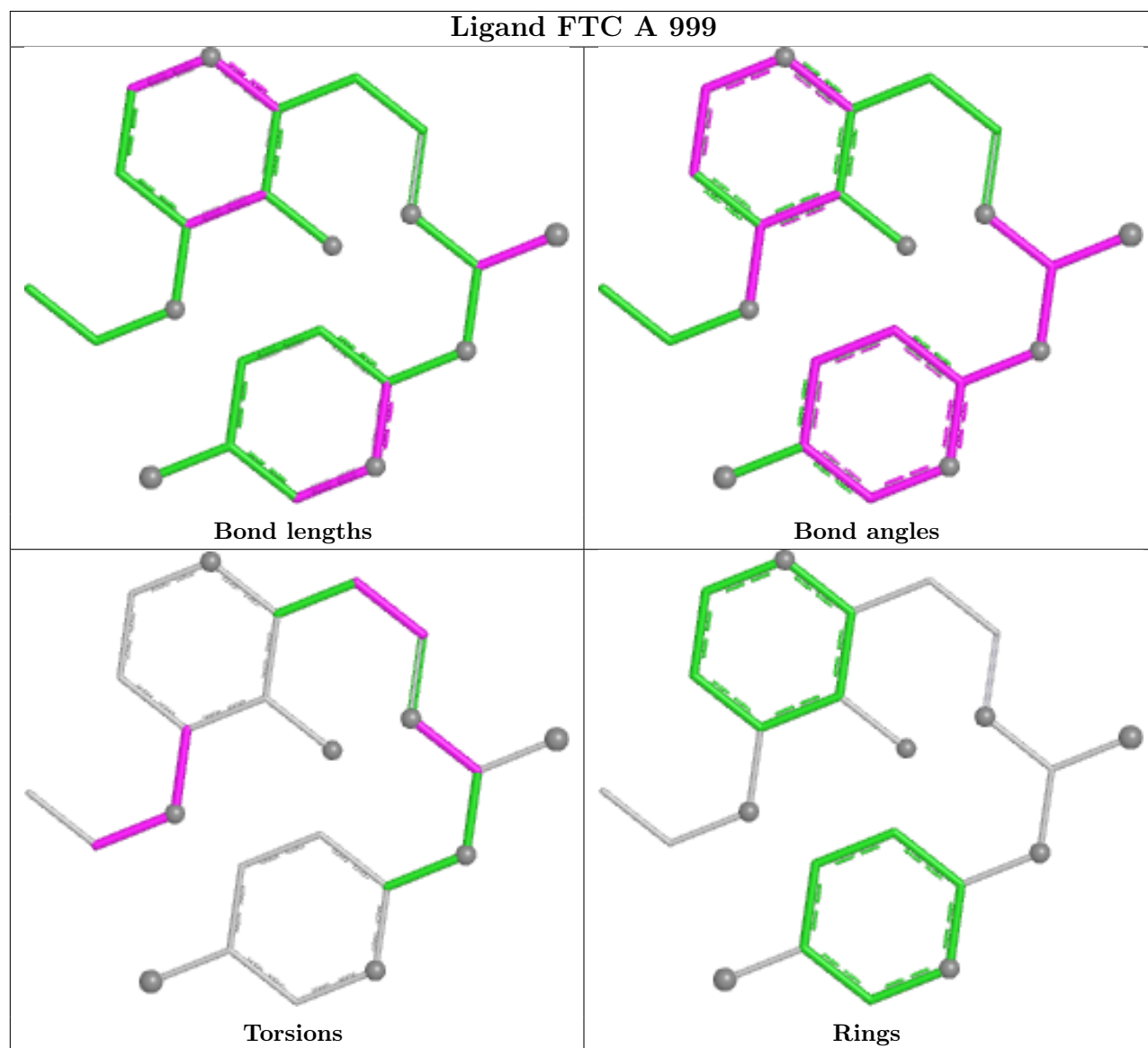
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	FTC	4	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.



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	A	534/560 (95%)	-0.37	1 (0%) 91 83	36, 84, 140, 150	0
2	B	402/440 (91%)	-0.45	0 100 100	37, 77, 136, 150	0
All	All	936/1000 (93%)	-0.40	1 (0%) 92 86	36, 81, 139, 150	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	280	8/9	0.97	0.06	56,70,77,85	0

6.3 Carbohydrates [i](#)

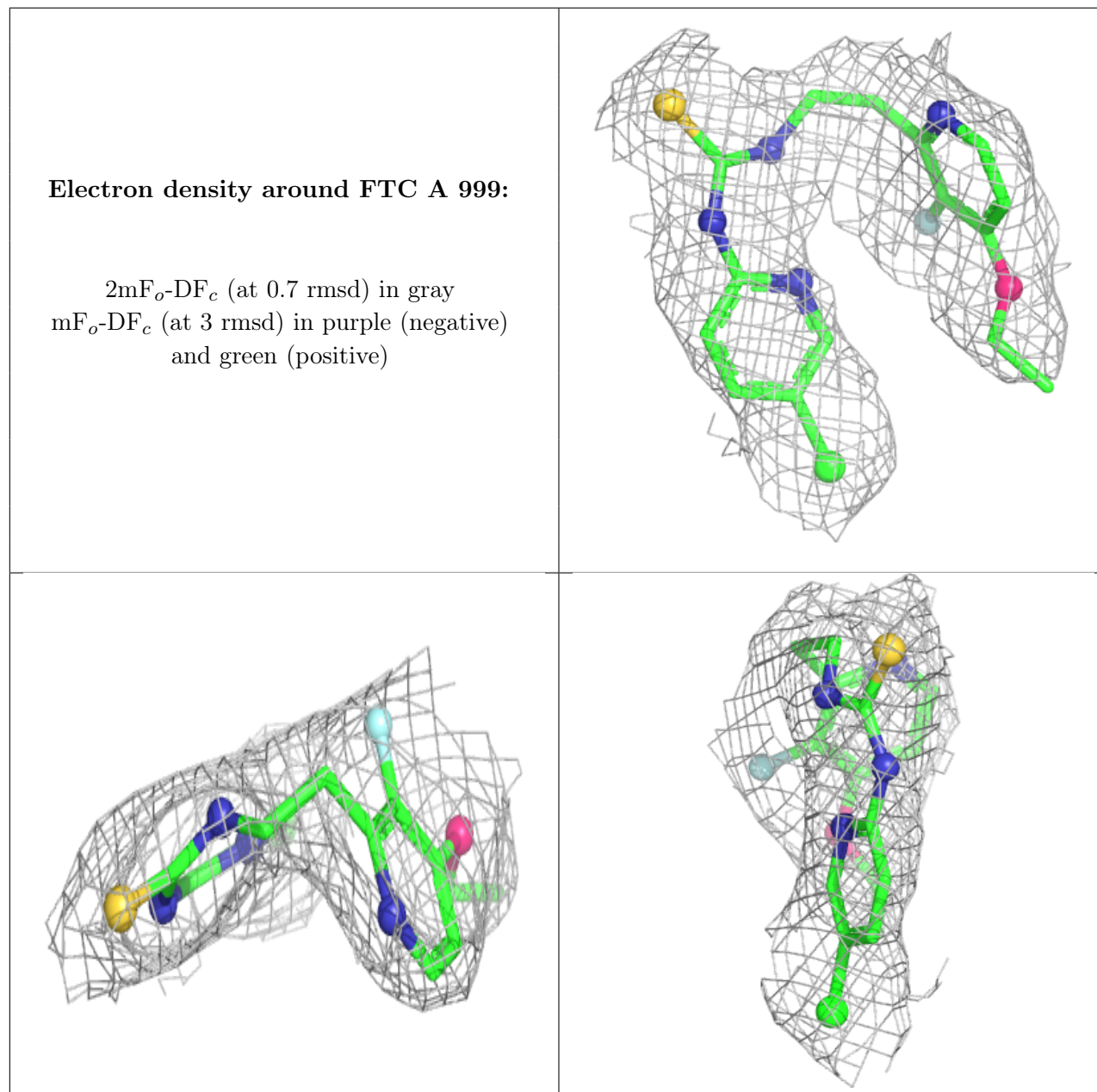
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	FTC	A	999	23/23	0.95	0.08	66,72,78,82	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.