



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:33 am GMT

PDB ID : 2R4O
Title : Crystal structure of the long-chain fatty acid transporter FadL mutant delta NPA
Authors : Hearn, E.M.; Patel, D.R.; Lepore, B.W.; Indic, M.; van den Berg, B.
Deposited on : 2007-08-31
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

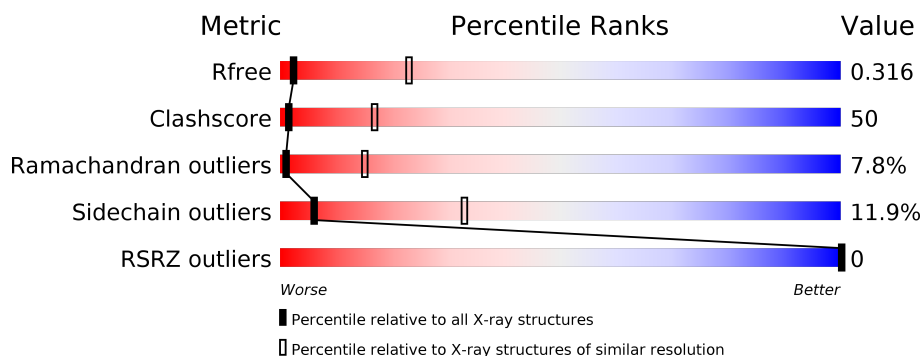
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	427	
1	B	427	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDA	A	501	-	-	-	X
2	LDA	A	503	-	-	X	X
2	LDA	B	502	-	-	-	X
2	LDA	B	504	-	-	X	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6550 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.

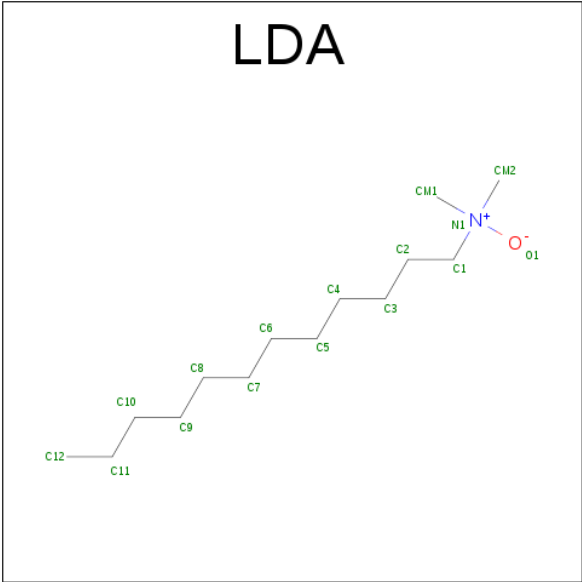
- Molecule 1 is a protein called Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3243	2049	551	637	6			
1	B	421	Total	C	N	O	S	0	0	0
			3243	2049	551	637	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	ASN	ENGINEERED	UNP P10384
A	34	GLY	PRO	ENGINEERED	UNP P10384
A	35	GLY	ALA	ENGINEERED	UNP P10384
A	197	THR	ILE	CONFLICT	UNP P10384
A	422	HIS	-	EXPRESSION TAG	UNP P10384
A	423	HIS	-	EXPRESSION TAG	UNP P10384
A	424	HIS	-	EXPRESSION TAG	UNP P10384
A	425	HIS	-	EXPRESSION TAG	UNP P10384
A	426	HIS	-	EXPRESSION TAG	UNP P10384
A	427	HIS	-	EXPRESSION TAG	UNP P10384
B	33	GLY	ASN	ENGINEERED	UNP P10384
B	34	GLY	PRO	ENGINEERED	UNP P10384
B	35	GLY	ALA	ENGINEERED	UNP P10384
B	197	THR	ILE	CONFLICT	UNP P10384
B	422	HIS	-	EXPRESSION TAG	UNP P10384
B	423	HIS	-	EXPRESSION TAG	UNP P10384
B	424	HIS	-	EXPRESSION TAG	UNP P10384
B	425	HIS	-	EXPRESSION TAG	UNP P10384
B	426	HIS	-	EXPRESSION TAG	UNP P10384
B	427	HIS	-	EXPRESSION TAG	UNP P10384

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

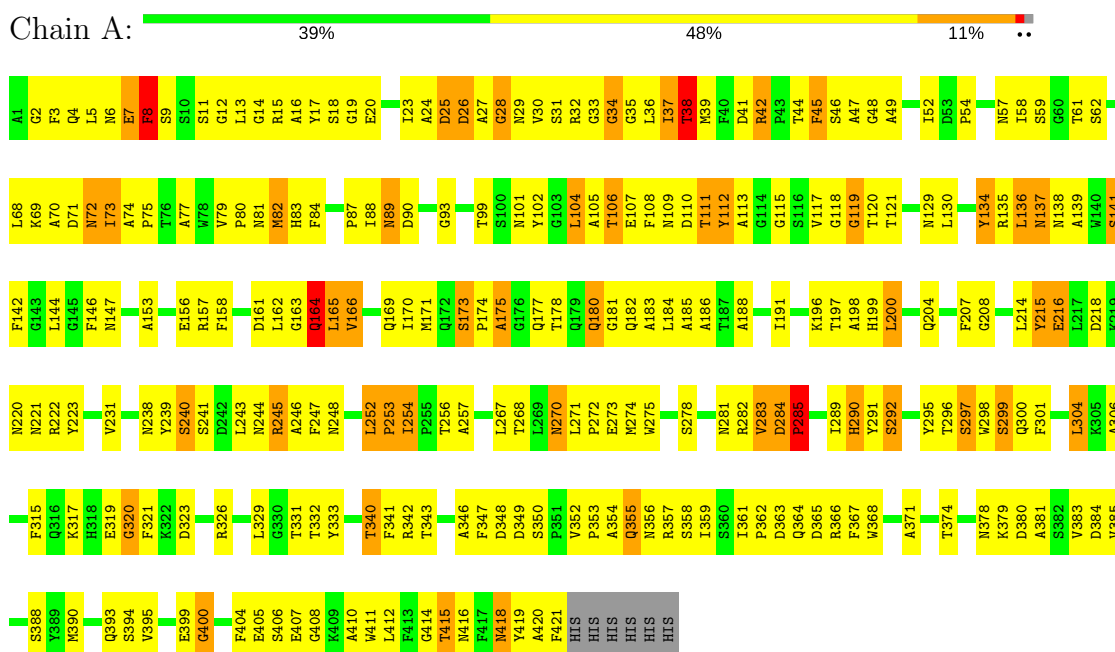


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		

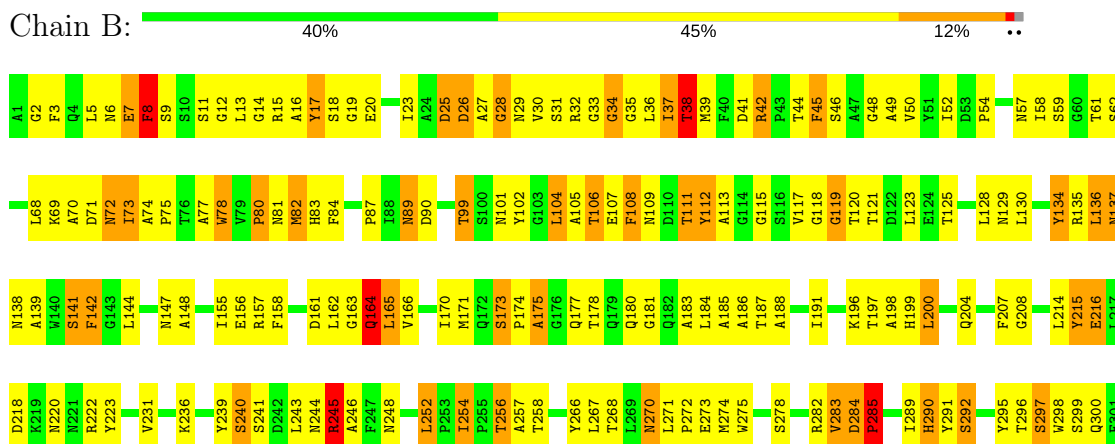
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Long-chain fatty acid transport protein



• Molecule 1: Long-chain fatty acid transport protein



D384	Q302	D394	Q303	D323	Q304	D329	Q305	D340	Q306	D330	Q307	D331	Q308	D332	Q309	D333	Q310	D334	Q311	D335	Q312	D336	Q313	D337	Q314	D338	Q315	D339	Q316	D340	Q317	D341	Q318	D342	Q319	D343	Q320	D344	Q321	D345	Q322	D346	Q323	D347	Q324	D348	Q325	D349	Q326	D350	Q327	D351	Q328	D352	Q329	D353	Q330	D354	Q331	D355	Q332	D356	Q333	D357	Q334	D358	Q335	D359	Q336	D360	Q337	D361	Q338	D362	Q339	D363	Q340	D364	Q341	D365	Q342	D366	Q343	D367	Q344	D368	Q345	D369	Q346	D370	Q347	D371	Q348	D372	Q349	D373	Q350	D374	Q351	D375	Q352	D376	Q353	D377	Q354	D378	Q355	D379	Q356	D380	Q357	D381	Q358	D382	Q359	D383	Q360	D384	Q361	D385	Q362	D386	Q363	D387	Q364	D388	Q365	D389	Q366	D390	Q367	D391	Q368	D392	Q369	D393	Q370	D394	Q371	D395	Q372	D396	Q373	D397	Q374	D398	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
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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	63.05Å 146.62Å 151.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.60 41.54 – 3.58	Depositor EDS
% Data completeness (in resolution range)	98.7 (10.00-3.60) 98.4 (41.54-3.58)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.314 0.250 , 0.316	Depositor DCC
R_{free} test set	1602 reflections (10.12%)	DCC
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 7.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for -h,l,k	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6550	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.49% 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: LDA

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	0.47	0/3331	0.72	0/4533
1	B	0.48	0/3331	0.73	0/4533
All	All	0.48	0/6662	0.73	0/9066

There are no bond length outliers.

There are no bond angle outliers.

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	3243	0	3020	313	0
1	B	3243	0	3020	320	0
2	A	32	0	62	14	0
2	B	32	0	62	12	0
All	All	6550	0	6164	635	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 50.

All (635) 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:346:ALA:HB3	1:B:368:TRP:HB2	1.37	1.05
1:B:75:PRO:HD2	1:B:105:ALA:HB1	1.39	1.05
1:A:75:PRO:HD2	1:A:105:ALA:HB1	1.38	1.04
1:A:346:ALA:HB3	1:A:368:TRP:HB2	1.38	1.04
1:B:89:ASN:CG	1:B:90:ASP:H	1.64	1.00
1:B:134:TYR:HD2	1:B:135:ARG:N	1.62	0.97
1:B:252:LEU:HD12	1:B:252:LEU:H	1.27	0.97
1:A:134:TYR:HD2	1:A:135:ARG:N	1.65	0.95
1:A:19:GLY:N	1:A:292:SER:HB2	1.82	0.95
1:A:252:LEU:HD12	1:A:252:LEU:H	1.28	0.94
1:B:241:SER:HB3	1:B:257:ALA:HA	1.47	0.94
1:A:89:ASN:CG	1:A:90:ASP:H	1.71	0.93
1:A:357:ARG:NH1	1:A:395:VAL:HB	1.82	0.93
1:B:357:ARG:NH1	1:B:395:VAL:HB	1.83	0.92
1:A:289:ILE:HG13	1:A:331:THR:HG22	1.53	0.91
1:B:52:ILE:HG12	1:B:412:LEU:HD22	1.52	0.91
1:B:102:TYR:OH	1:B:272:PRO:HG2	1.72	0.90
1:B:52:ILE:HB	1:B:77:ALA:HB3	1.54	0.90
1:A:241:SER:HB3	1:A:257:ALA:HA	1.52	0.90
1:B:134:TYR:HD2	1:B:135:ARG:H	1.19	0.90
1:B:19:GLY:N	1:B:292:SER:HB2	1.87	0.89
1:B:289:ILE:HG13	1:B:331:THR:HG22	1.55	0.89
1:A:385:VAL:HG22	1:A:415:THR:HG23	1.54	0.88
1:A:134:TYR:HD2	1:A:135:ARG:H	1.22	0.88
1:B:68:LEU:HD12	1:B:404:PHE:HE2	1.37	0.88
1:B:75:PRO:CD	1:B:105:ALA:HB1	2.03	0.88
1:A:248:ASN:HD21	1:A:257:ALA:H	1.21	0.87
1:A:52:ILE:HB	1:A:77:ALA:HB3	1.57	0.87
1:A:75:PRO:CD	1:A:105:ALA:HB1	2.04	0.86
1:B:385:VAL:HG22	1:B:415:THR:HG23	1.55	0.86
1:A:157:ARG:C	1:A:197:THR:HG22	1.95	0.85
1:A:173:SER:O	1:A:175:ALA:N	2.08	0.85
1:A:38:THR:HG21	1:A:141:SER:HB3	1.57	0.85
1:B:173:SER:O	1:B:175:ALA:N	2.09	0.84
1:B:137:ASN:ND2	1:B:139:ALA:H	1.75	0.84
1:A:68:LEU:HD12	1:A:404:PHE:HE2	1.41	0.84
1:B:68:LEU:HD12	1:B:404:PHE:CE2	2.13	0.83
1:B:104:LEU:HA	2:B:502:LDA:H62	1.62	0.82
1:A:284:ASP:OD1	1:A:285:PRO:HD2	1.79	0.82
1:B:248:ASN:HD21	1:B:257:ALA:H	1.25	0.82
1:B:117:VAL:HG13	1:B:359:ILE:HD11	1.61	0.82
1:A:31:SER:O	1:A:32:ARG:HB3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HG12	1:A:412:LEU:HD22	1.61	0.81
1:A:73:ILE:O	1:A:75:PRO:HD3	1.79	0.81
1:B:31:SER:O	1:B:32:ARG:HB3	1.80	0.80
1:B:157:ARG:C	1:B:197:THR:HG22	2.01	0.80
1:B:267:LEU:HD23	1:B:268:THR:N	1.96	0.80
1:A:111:THR:O	1:A:112:TYR:HB3	1.83	0.79
1:A:28:GLY:HA2	1:A:83:HIS:CG	2.17	0.79
1:B:273:GLU:HG2	1:B:297:SER:OG	1.82	0.78
1:A:137:ASN:ND2	1:A:139:ALA:H	1.81	0.78
1:B:28:GLY:HA2	1:B:83:HIS:CG	2.18	0.78
1:A:267:LEU:HD23	1:A:268:THR:N	1.99	0.77
1:B:12:GLY:HA2	1:B:15:ARG:NH1	1.99	0.77
1:A:68:LEU:HD12	1:A:404:PHE:CE2	2.18	0.77
1:B:111:THR:O	1:B:112:TYR:HB3	1.85	0.76
1:B:72:ASN:HD22	1:B:73:ILE:N	1.83	0.76
1:A:104:LEU:HB2	2:A:501:LDA:H21	1.67	0.76
1:A:72:ASN:HD22	1:A:73:ILE:N	1.84	0.76
1:B:89:ASN:CG	1:B:90:ASP:N	2.35	0.75
1:B:200:LEU:HB3	2:B:504:LDA:H111	1.67	0.75
1:B:141:SER:C	1:B:142:PHE:HD2	1.89	0.75
1:B:134:TYR:CD2	1:B:135:ARG:N	2.52	0.75
1:A:273:GLU:HG2	1:A:297:SER:OG	1.86	0.75
1:B:73:ILE:O	1:B:75:PRO:HD3	1.87	0.75
1:A:48:GLY:HA3	1:A:416:ASN:ND2	2.02	0.74
1:A:75:PRO:HD2	1:A:105:ALA:CB	2.18	0.74
1:A:157:ARG:O	1:A:197:THR:HG22	1.88	0.74
1:B:157:ARG:O	1:B:197:THR:HG22	1.88	0.74
1:A:156:GLU:OE1	1:A:196:LYS:HE2	1.88	0.73
1:B:241:SER:CB	1:B:257:ALA:HA	2.18	0.73
1:A:296:THR:O	1:A:298:TRP:N	2.22	0.73
1:A:317:LYS:NZ	2:A:503:LDA:HM23	2.04	0.73
1:B:38:THR:HG21	1:B:141:SER:HB3	1.69	0.72
1:A:102:TYR:OH	1:A:272:PRO:HG2	1.89	0.72
1:B:73:ILE:HG22	1:B:107:GLU:H	1.54	0.72
1:B:75:PRO:HD2	1:B:105:ALA:CB	2.19	0.72
1:A:23:ILE:HG12	1:A:23:ILE:O	1.90	0.72
1:B:346:ALA:HB3	1:B:368:TRP:CB	2.15	0.72
1:A:346:ALA:HB3	1:A:368:TRP:CB	2.17	0.72
1:A:12:GLY:HA2	1:A:15:ARG:NH1	2.05	0.71
1:A:62:SER:CB	1:A:68:LEU:HD21	2.20	0.71
1:B:62:SER:CB	1:B:68:LEU:HD21	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:TRP:O	1:A:412:LEU:HD23	1.91	0.71
1:A:270:ASN:N	1:A:270:ASN:HD22	1.89	0.70
1:A:134:TYR:CD2	1:A:135:ARG:N	2.55	0.70
1:A:58:ILE:HB	1:A:70:ALA:HB3	1.74	0.70
1:A:38:THR:HG21	1:A:141:SER:CB	2.22	0.70
1:B:48:GLY:HA3	1:B:416:ASN:ND2	2.05	0.70
1:B:73:ILE:HG22	1:B:107:GLU:N	2.07	0.70
1:A:248:ASN:ND2	1:A:257:ALA:H	1.90	0.69
1:A:37:ILE:O	1:A:39:MET:N	2.25	0.69
1:B:291:TYR:O	1:B:292:SER:HB2	1.92	0.69
1:A:89:ASN:CG	1:A:90:ASP:N	2.42	0.69
1:A:58:ILE:HD13	1:A:406:SER:HB2	1.75	0.69
1:B:199:HIS:O	1:B:239:TYR:HA	1.92	0.68
1:B:284:ASP:OD1	1:B:285:PRO:HD2	1.93	0.68
1:A:199:HIS:O	1:A:239:TYR:HA	1.93	0.68
1:B:156:GLU:OE1	1:B:196:LYS:HE2	1.93	0.68
1:A:248:ASN:HD21	1:A:257:ALA:N	1.90	0.68
1:B:166:VAL:O	1:B:170:ILE:HG13	1.93	0.68
1:B:200:LEU:N	1:B:200:LEU:HD12	2.09	0.68
1:B:384:ASP:HB2	1:B:416:ASN:HB2	1.74	0.68
1:A:46:SER:CB	1:A:418:ASN:HB3	2.24	0.67
1:B:420:ALA:C	1:B:421:PHE:HD2	1.96	0.67
1:B:248:ASN:HD21	1:B:256:THR:HA	1.59	0.67
1:B:267:LEU:HD23	1:B:267:LEU:C	2.14	0.67
1:A:358:SER:HB2	1:A:399:GLU:OE1	1.95	0.67
1:B:37:ILE:O	1:B:39:MET:N	2.28	0.67
1:B:214:LEU:HD12	1:B:215:TYR:N	2.10	0.67
1:A:248:ASN:HD21	1:A:256:THR:HA	1.57	0.67
1:B:38:THR:HG21	1:B:141:SER:CB	2.24	0.67
1:B:58:ILE:HB	1:B:70:ALA:HB3	1.76	0.67
1:B:46:SER:CB	1:B:418:ASN:HB3	2.25	0.67
1:A:141:SER:C	1:A:142:PHE:HD2	1.97	0.66
1:A:267:LEU:C	1:A:267:LEU:HD23	2.15	0.66
1:A:361:ILE:HD11	2:A:503:LDA:H21	1.75	0.66
1:A:220:ASN:HB3	1:A:282:ARG:HB3	1.76	0.66
1:A:102:TYR:CE1	1:A:271:LEU:HB3	2.31	0.66
1:A:166:VAL:O	1:A:170:ILE:HG13	1.94	0.66
1:B:220:ASN:HB3	1:B:282:ARG:HB3	1.77	0.66
1:A:252:LEU:CD1	1:A:252:LEU:H	2.04	0.66
1:A:200:LEU:N	1:A:200:LEU:HD12	2.12	0.65
1:A:243:LEU:HD13	1:A:254:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLY:O	1:B:35:GLY:N	2.28	0.65
1:A:7:GLU:O	1:A:9:SER:N	2.27	0.65
1:B:215:TYR:HD2	1:B:216:GLU:N	1.93	0.65
1:B:23:ILE:O	1:B:23:ILE:HG12	1.96	0.65
1:B:384:ASP:O	1:B:415:THR:HA	1.97	0.65
1:A:18:SER:O	1:A:290:HIS:HB2	1.96	0.65
1:A:304:LEU:HD21	2:A:503:LDA:H52	1.79	0.65
1:B:104:LEU:HD11	1:B:121:THR:HG22	1.78	0.65
1:B:46:SER:HB2	1:B:418:ASN:HB3	1.78	0.65
1:B:385:VAL:CG2	1:B:415:THR:HG23	2.24	0.65
1:B:62:SER:HB2	1:B:68:LEU:HD21	1.78	0.65
1:B:390:MET:HE2	1:B:412:LEU:HD11	1.79	0.64
1:B:183:ALA:O	1:B:186:ALA:HB3	1.97	0.64
1:B:243:LEU:HD13	1:B:254:ILE:HD11	1.79	0.64
1:A:385:VAL:CG2	1:A:415:THR:HG23	2.27	0.64
1:A:388:SER:HB2	1:A:412:LEU:HB2	1.80	0.64
1:B:248:ASN:HD21	1:B:257:ALA:N	1.94	0.64
1:A:304:LEU:HD13	2:A:503:LDA:HM13	1.80	0.64
1:A:243:LEU:CD1	1:A:254:ILE:HD11	2.28	0.63
1:B:296:THR:O	1:B:298:TRP:N	2.31	0.63
1:A:107:GLU:O	1:A:108:PHE:HB2	1.98	0.63
1:A:46:SER:HB2	1:A:418:ASN:HB3	1.81	0.63
1:B:388:SER:HB2	1:B:412:LEU:HB2	1.81	0.63
1:A:215:TYR:HD2	1:A:216:GLU:N	1.97	0.63
1:B:81:ASN:HD21	1:B:416:ASN:HD21	1.47	0.63
1:A:62:SER:HB2	1:A:68:LEU:HD21	1.80	0.63
1:B:270:ASN:N	1:B:270:ASN:HD22	1.95	0.63
1:B:73:ILE:H	1:B:73:ILE:HD12	1.64	0.63
1:A:104:LEU:HD11	1:A:121:THR:HG22	1.81	0.62
1:A:326:ARG:HG3	1:A:348:ASP:HB3	1.80	0.62
1:A:117:VAL:HG13	1:A:359:ILE:HD11	1.81	0.62
1:A:33:GLY:O	1:A:35:GLY:N	2.33	0.62
1:A:216:GLU:HB3	1:A:222:ARG:HG2	1.80	0.62
1:A:248:ASN:ND2	1:A:256:THR:HA	2.15	0.62
1:B:30:VAL:HG13	1:B:31:SER:N	2.15	0.62
1:A:317:LYS:HZ1	2:A:503:LDA:HM23	1.62	0.61
1:B:248:ASN:ND2	1:B:257:ALA:H	1.97	0.61
1:B:420:ALA:O	1:B:421:PHE:HD2	1.82	0.61
1:B:18:SER:O	1:B:290:HIS:HB2	2.00	0.61
1:A:30:VAL:HG13	1:A:31:SER:N	2.15	0.61
1:A:384:ASP:HB2	1:A:416:ASN:HB2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LEU:HA	1:B:165:LEU:CD1	2.30	0.61
1:A:183:ALA:O	1:A:186:ALA:HB3	2.00	0.61
1:A:57:ASN:HB2	1:A:407:GLU:HG3	1.82	0.61
1:A:291:TYR:O	1:A:292:SER:HB2	2.01	0.61
1:B:137:ASN:ND2	1:B:137:ASN:C	2.53	0.61
1:B:291:TYR:O	1:B:292:SER:CB	2.49	0.60
1:B:117:VAL:HG21	1:B:399:GLU:CD	2.22	0.60
1:A:241:SER:CB	1:A:257:ALA:HA	2.26	0.60
1:B:19:GLY:H	1:B:292:SER:HB2	1.66	0.60
1:B:248:ASN:ND2	1:B:256:THR:HA	2.15	0.60
1:B:32:ARG:O	1:B:32:ARG:HG2	2.00	0.60
1:B:48:GLY:HA3	1:B:416:ASN:HD22	1.66	0.60
1:A:105:ALA:O	1:A:106:THR:HB	2.01	0.60
1:A:304:LEU:HD22	2:A:503:LDA:HM13	1.84	0.60
1:B:107:GLU:O	1:B:108:PHE:HB2	2.01	0.60
1:B:222:ARG:C	1:B:223:TYR:CD1	2.75	0.60
1:A:222:ARG:C	1:A:223:TYR:CD1	2.75	0.60
1:A:19:GLY:H	1:A:292:SER:HB2	1.62	0.60
1:A:48:GLY:HA3	1:A:416:ASN:HD22	1.66	0.60
1:B:135:ARG:O	1:B:136:LEU:C	2.40	0.60
1:A:252:LEU:N	1:A:252:LEU:HD12	2.10	0.60
1:A:420:ALA:C	1:A:421:PHE:HD2	2.04	0.60
1:B:16:ALA:O	1:B:17:TYR:C	2.40	0.60
1:B:411:TRP:O	1:B:412:LEU:HD23	2.02	0.59
1:A:11:SER:HB3	1:A:384:ASP:OD1	2.02	0.59
1:A:384:ASP:O	1:A:415:THR:HA	2.02	0.59
1:B:7:GLU:CD	1:B:7:GLU:H	2.04	0.59
1:B:105:ALA:O	1:B:106:THR:HB	2.02	0.59
1:A:117:VAL:HG21	1:A:399:GLU:CD	2.23	0.59
1:A:41:ASP:O	1:A:87:PRO:HG3	2.02	0.59
1:A:385:VAL:HA	1:A:414:GLY:O	2.03	0.59
1:A:420:ALA:O	1:A:421:PHE:HD2	1.85	0.59
1:A:73:ILE:HG22	1:A:107:GLU:H	1.67	0.59
1:B:385:VAL:HA	1:B:414:GLY:O	2.02	0.59
1:B:7:GLU:O	1:B:9:SER:N	2.30	0.59
1:A:137:ASN:C	1:A:137:ASN:ND2	2.56	0.58
1:A:135:ARG:O	1:A:136:LEU:C	2.41	0.58
1:A:33:GLY:HA3	1:A:36:LEU:HD23	1.84	0.58
1:B:57:ASN:HB2	1:B:407:GLU:HG3	1.86	0.58
1:B:142:PHE:N	1:B:142:PHE:HD2	2.02	0.58
1:A:358:SER:CB	1:A:399:GLU:OE1	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLU:H	1:A:300:GLN:HE22	1.52	0.58
1:A:37:ILE:C	1:A:39:MET:H	2.07	0.58
1:B:216:GLU:HB3	1:B:222:ARG:HG2	1.86	0.58
1:B:41:ASP:O	1:B:87:PRO:HG3	2.03	0.58
1:A:332:THR:HG23	1:A:341:PHE:O	2.03	0.58
1:A:72:ASN:HD22	1:A:73:ILE:H	1.50	0.58
1:B:142:PHE:N	1:B:142:PHE:CD2	2.71	0.58
1:B:326:ARG:HG3	1:B:348:ASP:HB3	1.86	0.57
1:B:361:ILE:HD11	2:B:504:LDA:O1	2.04	0.57
1:B:37:ILE:C	1:B:39:MET:H	2.08	0.57
1:A:214:LEU:HD12	1:A:215:TYR:N	2.19	0.57
1:B:359:ILE:HG12	1:B:399:GLU:OE2	2.04	0.57
1:A:73:ILE:H	1:A:73:ILE:HD12	1.69	0.57
1:B:252:LEU:N	1:B:252:LEU:HD12	2.08	0.57
1:B:352:VAL:HG21	1:B:357:ARG:HA	1.87	0.57
1:A:142:PHE:CD2	1:A:142:PHE:N	2.73	0.57
1:B:2:GLY:O	1:B:366:ARG:NH2	2.37	0.57
1:A:38:THR:OG1	1:A:135:ARG:NH1	2.37	0.57
1:A:13:LEU:HA	1:A:17:TYR:CZ	2.40	0.57
1:A:32:ARG:HG2	1:A:32:ARG:O	2.03	0.57
1:B:129:ASN:OD1	1:B:130:LEU:N	2.38	0.57
1:B:6:ASN:O	1:B:8:PHE:HD1	1.88	0.57
1:A:299:SER:OG	1:A:323:ASP:OD2	2.23	0.57
1:A:162:LEU:HA	1:A:165:LEU:CD1	2.34	0.56
1:B:30:VAL:CG1	1:B:31:SER:N	2.68	0.56
1:A:15:ARG:NH1	1:A:20:GLU:OE2	2.38	0.56
1:A:378:ASN:C	1:A:380:ASP:H	2.08	0.56
1:B:113:ALA:HB1	1:B:161:ASP:CG	2.25	0.56
1:A:73:ILE:HG22	1:A:107:GLU:N	2.19	0.56
1:B:134:TYR:CD2	1:B:136:LEU:N	2.72	0.56
1:B:50:VAL:O	1:B:78:TRP:O	2.23	0.56
1:A:25:ASP:O	1:A:26:ASP:CB	2.53	0.56
1:A:88:ILE:HG13	1:A:93:GLY:HA2	1.88	0.56
1:B:105:ALA:H	2:B:502:LDA:H51	1.70	0.56
1:B:52:ILE:HG12	1:B:412:LEU:CD2	2.32	0.56
1:B:33:GLY:HA3	1:B:36:LEU:HD23	1.88	0.56
1:B:358:SER:HB2	1:B:399:GLU:OE1	2.05	0.56
1:A:289:ILE:HG12	1:A:290:HIS:N	2.20	0.56
1:A:394:SER:OG	1:A:407:GLU:HB3	2.06	0.56
1:A:134:TYR:CD2	1:A:136:LEU:N	2.74	0.55
1:A:199:HIS:C	1:A:200:LEU:HD12	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLN:CD	1:A:355:GLN:H	2.10	0.55
1:B:162:LEU:HA	1:B:165:LEU:HD13	1.89	0.55
1:A:352:VAL:HG21	1:A:357:ARG:HA	1.88	0.55
1:B:117:VAL:HG22	1:B:117:VAL:O	2.06	0.55
1:B:58:ILE:HD13	1:B:406:SER:HB2	1.88	0.55
1:B:399:GLU:O	1:B:400:GLY:C	2.45	0.55
1:A:274:MET:HG3	1:A:295:TYR:O	2.06	0.55
1:B:123:LEU:HB2	2:B:504:LDA:H31	1.88	0.55
1:B:113:ALA:HA	1:B:161:ASP:H	1.71	0.55
1:A:117:VAL:O	1:A:359:ILE:HD11	2.06	0.55
1:B:111:THR:O	1:B:112:TYR:CB	2.55	0.55
1:B:239:TYR:CG	1:B:240:SER:N	2.74	0.55
1:B:25:ASP:O	1:B:26:ASP:CB	2.55	0.55
1:A:135:ARG:HG2	1:A:135:ARG:O	2.07	0.55
1:B:243:LEU:CD1	1:B:254:ILE:HD11	2.36	0.55
1:B:72:ASN:HD22	1:B:73:ILE:H	1.53	0.55
1:B:394:SER:OG	1:B:407:GLU:HB3	2.07	0.54
1:A:13:LEU:HB2	1:A:17:TYR:OH	2.06	0.54
1:A:52:ILE:HG23	1:A:412:LEU:CD2	2.36	0.54
1:A:129:ASN:OD1	1:A:130:LEU:N	2.40	0.54
1:A:142:PHE:HD2	1:A:142:PHE:N	2.05	0.54
1:A:291:TYR:O	1:A:292:SER:CB	2.55	0.54
1:B:25:ASP:OD1	1:B:25:ASP:O	2.25	0.54
1:B:354:ALA:HA	1:B:357:ARG:HG3	1.89	0.54
1:B:52:ILE:HG21	2:B:502:LDA:HM11	1.89	0.54
1:A:378:ASN:O	1:A:380:ASP:N	2.41	0.54
1:A:104:LEU:CD1	1:A:104:LEU:C	2.75	0.54
1:B:54:PRO:HG2	1:B:74:ALA:O	2.07	0.54
1:A:19:GLY:CA	1:A:292:SER:HB2	2.36	0.54
1:A:30:VAL:CG1	1:A:31:SER:N	2.70	0.54
1:B:214:LEU:HD12	1:B:215:TYR:H	1.71	0.54
1:B:289:ILE:HG12	1:B:290:HIS:N	2.22	0.54
1:A:113:ALA:HA	1:A:161:ASP:H	1.72	0.54
1:A:162:LEU:O	1:A:165:LEU:HD12	2.08	0.54
1:B:218:ASP:OD1	1:B:220:ASN:N	2.37	0.54
1:B:11:SER:HB3	1:B:384:ASP:OD1	2.08	0.54
1:B:28:GLY:O	1:B:30:VAL:N	2.35	0.54
1:A:111:THR:O	1:A:112:TYR:CB	2.53	0.54
1:B:191:ILE:N	1:B:191:ILE:HD12	2.23	0.54
1:A:74:ALA:HA	1:A:105:ALA:HB1	1.91	0.53
1:A:58:ILE:CD1	1:A:406:SER:HB2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ALA:HB1	1:A:161:ASP:CG	2.29	0.53
1:A:59:SER:OG	1:A:405:GLU:HB3	2.09	0.53
1:A:52:ILE:HG23	1:A:412:LEU:HD21	1.89	0.53
1:A:28:GLY:O	1:A:30:VAL:N	2.34	0.53
1:B:137:ASN:HD22	1:B:137:ASN:C	2.12	0.53
1:B:378:ASN:C	1:B:380:ASP:H	2.12	0.53
1:B:13:LEU:HA	1:B:17:TYR:CZ	2.44	0.53
1:B:102:TYR:CE1	1:B:271:LEU:HB3	2.44	0.53
1:A:117:VAL:HG22	1:A:117:VAL:O	2.08	0.53
1:B:17:TYR:HA	1:B:20:GLU:CD	2.30	0.52
1:B:181:GLY:O	1:B:185:ALA:N	2.32	0.52
1:A:162:LEU:HA	1:A:165:LEU:HD13	1.92	0.52
1:B:274:MET:HG3	1:B:295:TYR:O	2.09	0.52
1:B:61:THR:CA	1:B:68:LEU:HD23	2.40	0.52
1:B:273:GLU:H	1:B:300:GLN:HE22	1.58	0.52
1:B:319:GLU:O	1:B:320:GLY:C	2.48	0.52
1:A:2:GLY:O	1:A:366:ARG:NH2	2.42	0.52
1:A:161:ASP:O	1:A:164:GLN:HB2	2.10	0.52
1:A:107:GLU:O	1:A:119:GLY:O	2.28	0.52
1:A:14:GLY:HA3	1:A:342:ARG:HD2	1.92	0.52
1:A:16:ALA:O	1:A:17:TYR:C	2.48	0.52
1:B:130:LEU:C	1:B:130:LEU:HD23	2.30	0.52
1:B:38:THR:OG1	1:B:135:ARG:NH1	2.42	0.52
1:B:147:ASN:HB2	1:B:208:GLY:O	2.09	0.52
1:B:243:LEU:O	1:B:257:ALA:HB1	2.10	0.52
1:B:14:GLY:HA3	1:B:342:ARG:HD2	1.92	0.52
1:B:349:ASP:OD1	1:B:365:ASP:OD1	2.28	0.52
1:B:135:ARG:HG2	1:B:135:ARG:O	2.10	0.52
1:A:239:TYR:CG	1:A:240:SER:N	2.78	0.51
1:A:349:ASP:OD1	1:A:365:ASP:OD1	2.27	0.51
1:A:399:GLU:O	1:A:400:GLY:C	2.48	0.51
1:B:191:ILE:HG22	1:B:191:ILE:O	2.11	0.51
1:B:364:GLN:O	1:B:365:ASP:C	2.48	0.51
1:A:185:ALA:O	1:A:188:ALA:HB3	2.10	0.51
1:A:353:PRO:HB2	1:A:355:GLN:NE2	2.26	0.51
1:B:49:ALA:HA	1:B:80:PRO:HA	1.91	0.51
1:A:130:LEU:HD23	1:A:130:LEU:C	2.31	0.51
1:A:54:PRO:HG2	1:A:74:ALA:O	2.10	0.51
1:A:161:ASP:N	1:A:161:ASP:OD1	2.41	0.51
1:A:191:ILE:HD12	1:A:191:ILE:N	2.26	0.51
1:A:19:GLY:N	1:A:292:SER:CB	2.66	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:THR:CA	1:A:68:LEU:HD23	2.41	0.51
1:B:15:ARG:HG3	1:B:15:ARG:HH11	1.75	0.51
1:A:23:ILE:O	1:A:23:ILE:HG23	2.10	0.51
1:A:354:ALA:HA	1:A:357:ARG:HG3	1.92	0.51
1:B:204:GLN:NE2	1:B:204:GLN:HA	2.26	0.51
1:A:19:GLY:H	1:A:292:SER:CB	2.23	0.51
1:B:52:ILE:HG23	1:B:412:LEU:HD21	1.92	0.50
1:A:104:LEU:C	1:A:104:LEU:HD12	2.32	0.50
1:A:191:ILE:O	1:A:191:ILE:HG22	2.11	0.50
1:A:37:ILE:C	1:A:39:MET:N	2.65	0.50
1:A:61:THR:C	1:A:68:LEU:HD23	2.32	0.50
1:A:273:GLU:CG	1:A:297:SER:OG	2.58	0.50
1:A:381:ALA:HA	1:A:418:ASN:O	2.11	0.50
1:A:317:LYS:HZ2	2:A:503:LDA:HM23	1.76	0.50
1:B:136:LEU:CD2	1:B:137:ASN:N	2.74	0.50
1:B:358:SER:CB	1:B:399:GLU:OE1	2.58	0.50
1:A:204:GLN:NE2	1:A:204:GLN:HA	2.27	0.50
1:A:6:ASN:O	1:A:8:PHE:HD1	1.94	0.50
1:B:19:GLY:H	1:B:292:SER:CB	2.25	0.50
1:B:117:VAL:O	1:B:359:ILE:HD11	2.11	0.50
1:A:104:LEU:HD12	1:A:104:LEU:O	2.12	0.50
1:A:218:ASP:OD1	1:A:220:ASN:N	2.43	0.50
1:B:120:THR:HG22	1:B:121:THR:N	2.26	0.50
1:B:161:ASP:O	1:B:164:GLN:HB2	2.12	0.50
1:A:81:ASN:HD21	1:A:416:ASN:HD21	1.58	0.49
1:B:104:LEU:HD11	1:B:121:THR:CG2	2.41	0.49
1:B:199:HIS:C	1:B:200:LEU:HD12	2.32	0.49
1:B:282:ARG:O	1:B:283:VAL:C	2.50	0.49
1:B:378:ASN:O	1:B:380:ASP:N	2.44	0.49
1:A:359:ILE:O	1:A:362:PRO:HD3	2.12	0.49
1:B:104:LEU:CD1	1:B:104:LEU:C	2.81	0.49
1:B:381:ALA:HA	1:B:418:ASN:O	2.11	0.49
1:A:181:GLY:O	1:A:185:ALA:N	2.39	0.49
1:B:252:LEU:HD13	1:B:254:ILE:CG2	2.43	0.49
1:A:11:SER:CB	1:A:26:ASP:OD1	2.61	0.49
1:B:27:ALA:HB2	1:B:44:THR:HB	1.95	0.49
1:A:49:ALA:HA	1:A:80:PRO:HA	1.94	0.49
1:B:215:TYR:C	1:B:215:TYR:CD2	2.86	0.49
1:B:420:ALA:C	1:B:421:PHE:CD2	2.83	0.49
1:A:25:ASP:O	1:A:26:ASP:CG	2.51	0.49
1:B:161:ASP:N	1:B:161:ASP:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HD22	1:B:68:LEU:N	2.28	0.49
1:B:52:ILE:HG23	1:B:412:LEU:CD2	2.43	0.49
1:A:120:THR:HG22	1:A:121:THR:N	2.28	0.49
1:A:329:LEU:HD23	1:A:329:LEU:C	2.33	0.49
1:A:353:PRO:HB2	1:A:355:GLN:OE1	2.13	0.49
1:B:89:ASN:ND2	1:B:90:ASP:H	2.10	0.49
1:A:290:HIS:ND1	1:A:290:HIS:N	2.61	0.48
1:B:162:LEU:O	1:B:165:LEU:HD12	2.13	0.48
1:B:62:SER:N	1:B:68:LEU:CD2	2.76	0.48
1:B:273:GLU:CG	1:B:297:SER:OG	2.57	0.48
1:A:221:ASN:ND2	1:A:281:ASN:HD22	2.11	0.48
1:B:119:GLY:HA3	1:B:157:ARG:HA	1.96	0.48
1:B:181:GLY:HA2	1:B:184:LEU:HB3	1.94	0.48
1:B:31:SER:O	1:B:32:ARG:CB	2.56	0.48
1:B:359:ILE:HA	1:B:362:PRO:HG3	1.95	0.48
2:B:504:LDA:H41	2:B:504:LDA:HM11	1.95	0.48
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.78	0.48
1:A:25:ASP:OD1	1:A:25:ASP:O	2.31	0.48
1:A:200:LEU:HD21	1:A:315:PHE:CD2	2.49	0.48
1:A:364:GLN:NE2	1:A:408:GLY:HA3	2.29	0.48
1:B:59:SER:OG	1:B:405:GLU:HB3	2.14	0.48
1:B:239:TYR:OH	1:B:256:THR:O	2.21	0.48
1:B:11:SER:CB	1:B:26:ASP:OD1	2.62	0.48
1:B:245:ARG:NH2	1:B:258:THR:O	2.46	0.48
1:B:364:GLN:NE2	1:B:408:GLY:HA3	2.29	0.48
1:B:37:ILE:C	1:B:39:MET:N	2.65	0.48
1:A:105:ALA:O	1:A:121:THR:O	2.31	0.48
1:B:304:LEU:HD21	2:B:504:LDA:HM11	1.96	0.48
1:A:137:ASN:C	1:A:137:ASN:HD22	2.17	0.48
1:B:137:ASN:HD21	1:B:139:ALA:H	1.59	0.48
1:B:252:LEU:HB2	1:B:254:ILE:HG22	1.96	0.48
1:A:147:ASN:HB2	1:A:208:GLY:O	2.13	0.47
1:A:215:TYR:CD2	1:A:215:TYR:C	2.85	0.47
1:B:74:ALA:HA	1:B:105:ALA:HB1	1.96	0.47
1:A:270:ASN:N	1:A:270:ASN:ND2	2.60	0.47
1:A:5:LEU:HB3	1:A:7:GLU:HG2	1.95	0.47
1:B:185:ALA:O	1:B:188:ALA:HB3	2.15	0.47
1:B:19:GLY:N	1:B:292:SER:CB	2.69	0.47
1:B:14:GLY:HA3	1:B:342:ARG:CD	2.45	0.47
1:A:6:ASN:O	1:A:7:GLU:C	2.53	0.47
1:B:109:ASN:C	1:B:111:THR:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLU:N	1:B:7:GLU:CD	2.67	0.47
1:A:31:SER:O	1:A:32:ARG:CB	2.54	0.47
1:A:7:GLU:H	1:A:7:GLU:CD	2.17	0.47
1:A:340:THR:HB	1:A:374:THR:HB	1.97	0.47
1:A:105:ALA:H	2:A:501:LDA:C2	2.28	0.47
1:B:290:HIS:N	1:B:290:HIS:ND1	2.63	0.47
1:B:346:ALA:CB	1:B:368:TRP:HB2	2.25	0.47
1:A:158:PHE:HA	1:A:197:THR:H	1.80	0.47
1:A:36:LEU:O	1:A:37:ILE:C	2.53	0.47
1:A:45:PHE:CD1	1:A:45:PHE:C	2.87	0.47
1:A:74:ALA:HA	1:A:105:ALA:CB	2.45	0.47
1:A:297:SER:HA	1:A:323:ASP:OD2	2.15	0.47
1:A:359:ILE:HA	1:A:362:PRO:HG3	1.95	0.47
1:A:364:GLN:O	1:A:365:ASP:C	2.53	0.47
1:B:340:THR:HB	1:B:374:THR:HB	1.97	0.47
1:B:61:THR:C	1:B:68:LEU:HD23	2.35	0.47
1:A:26:ASP:C	1:A:26:ASP:OD2	2.53	0.47
1:B:30:VAL:O	1:B:34:GLY:N	2.42	0.47
1:A:118:GLY:O	1:A:119:GLY:C	2.54	0.46
1:A:356:ASN:O	1:A:357:ARG:C	2.54	0.46
1:A:353:PRO:HB2	1:A:355:GLN:HE22	1.79	0.46
1:A:79:VAL:HG22	2:A:501:LDA:H112	1.96	0.46
1:B:120:THR:CG2	1:B:121:THR:N	2.78	0.46
1:A:136:LEU:CD2	1:A:137:ASN:N	2.79	0.46
1:B:19:GLY:CA	1:B:292:SER:HB2	2.45	0.46
1:A:115:GLY:C	1:A:117:VAL:N	2.67	0.46
1:A:319:GLU:O	1:A:320:GLY:C	2.52	0.46
1:B:352:VAL:HG11	1:B:363:ASP:HB3	1.97	0.46
1:A:62:SER:N	1:A:68:LEU:CD2	2.79	0.46
1:A:68:LEU:N	1:A:68:LEU:HD22	2.31	0.46
1:B:105:ALA:O	1:B:121:THR:O	2.33	0.46
1:B:196:LYS:HD3	1:B:199:HIS:HB2	1.95	0.46
1:A:361:ILE:HD11	2:A:503:LDA:HM21	1.97	0.46
1:A:367:PHE:O	1:A:390:MET:HA	2.16	0.46
1:B:244:ASN:O	1:B:246:ALA:N	2.49	0.46
1:B:223:TYR:HA	1:B:278:SER:O	2.16	0.46
1:B:356:ASN:O	1:B:357:ARG:C	2.54	0.46
1:A:104:LEU:HD11	1:A:121:THR:CG2	2.45	0.46
1:A:181:GLY:HA2	1:A:184:LEU:HB3	1.97	0.46
1:B:156:GLU:O	1:B:157:ARG:HD3	2.16	0.46
1:B:399:GLU:O	1:B:400:GLY:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:SER:OG	1:B:323:ASP:OD2	2.34	0.46
1:A:106:THR:O	1:A:106:THR:HG22	2.16	0.46
1:A:162:LEU:O	1:A:163:GLY:C	2.54	0.46
1:A:134:TYR:CE2	1:A:136:LEU:HA	2.51	0.45
1:B:48:GLY:O	1:B:81:ASN:N	2.40	0.45
1:B:101:ASN:O	1:B:102:TYR:CG	2.69	0.45
1:B:136:LEU:HD22	1:B:137:ASN:HB3	1.97	0.45
1:B:162:LEU:O	1:B:163:GLY:C	2.54	0.45
1:B:267:LEU:HD23	1:B:268:THR:CA	2.47	0.45
1:A:15:ARG:HD3	1:A:290:HIS:HE2	1.82	0.45
1:B:359:ILE:O	1:B:362:PRO:HD3	2.17	0.45
1:B:6:ASN:O	1:B:7:GLU:C	2.55	0.45
1:A:34:GLY:O	1:A:37:ILE:HG13	2.17	0.45
1:A:30:VAL:O	1:A:34:GLY:N	2.43	0.45
1:A:14:GLY:HA3	1:A:342:ARG:CD	2.47	0.45
1:B:69:LYS:HE2	1:B:71:ASP:OD1	2.17	0.45
1:A:4:GLN:HA	1:A:102:TYR:CD2	2.51	0.45
1:B:155:ILE:HD11	2:B:504:LDA:H61	1.99	0.45
1:B:302:GLN:NE2	1:B:320:GLY:HA2	2.31	0.45
1:A:109:ASN:C	1:A:111:THR:H	2.19	0.45
1:A:282:ARG:O	1:A:283:VAL:C	2.55	0.45
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.82	0.45
1:A:73:ILE:HG21	1:A:108:PHE:CD1	2.52	0.45
1:B:104:LEU:C	1:B:104:LEU:HD12	2.38	0.45
1:B:135:ARG:HG3	1:B:135:ARG:HH11	1.82	0.45
1:B:239:TYR:O	1:B:240:SER:CB	2.65	0.45
1:A:347:PHE:CG	1:A:348:ASP:N	2.85	0.44
1:B:239:TYR:O	1:B:240:SER:HB3	2.16	0.44
1:A:164:GLN:O	1:A:165:LEU:C	2.56	0.44
1:A:57:ASN:O	1:A:406:SER:HA	2.16	0.44
1:B:352:VAL:CG1	1:B:363:ASP:HB3	2.48	0.44
1:A:136:LEU:HD22	1:A:137:ASN:HB3	2.00	0.44
1:A:352:VAL:HG11	1:A:363:ASP:HB3	1.99	0.44
1:B:236:LYS:HD3	1:B:266:TYR:CE2	2.53	0.44
1:B:25:ASP:O	1:B:26:ASP:CG	2.56	0.44
1:B:81:ASN:O	1:B:82:MET:HB2	2.18	0.44
1:A:120:THR:CG2	1:A:121:THR:N	2.80	0.44
1:A:346:ALA:CB	1:A:368:TRP:HB2	2.27	0.44
1:B:109:ASN:O	1:B:111:THR:O	2.36	0.44
1:B:156:GLU:HA	1:B:198:ALA:O	2.18	0.44
1:B:26:ASP:OD2	1:B:26:ASP:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:TYR:CG	1:A:271:LEU:HD22	2.52	0.44
1:A:304:LEU:HD13	2:A:503:LDA:CM1	2.48	0.44
1:A:348:ASP:O	1:A:348:ASP:OD2	2.35	0.44
1:B:134:TYR:CE2	1:B:136:LEU:HA	2.53	0.44
1:B:164:GLN:O	1:B:165:LEU:C	2.57	0.44
1:B:266:TYR:HB2	1:B:307:THR:HG23	2.00	0.44
1:A:178:THR:C	1:A:180:GLN:N	2.71	0.44
1:B:332:THR:HG23	1:B:341:PHE:O	2.17	0.44
1:A:119:GLY:HA3	1:A:157:ARG:HA	2.00	0.43
1:A:223:TYR:HA	1:A:278:SER:O	2.18	0.43
1:B:178:THR:C	1:B:180:GLN:N	2.71	0.43
1:B:15:ARG:NH1	1:B:20:GLU:OE2	2.51	0.43
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.83	0.43
1:A:165:LEU:O	1:A:166:VAL:C	2.56	0.43
1:A:267:LEU:HD12	1:A:306:ALA:HB2	2.00	0.43
1:A:352:VAL:CG1	1:A:363:ASP:HB3	2.49	0.43
1:B:282:ARG:HG3	1:B:282:ARG:O	2.17	0.43
1:B:353:PRO:HB2	1:B:355:GLN:NE2	2.32	0.43
1:B:129:ASN:OD1	1:B:129:ASN:C	2.56	0.43
1:A:135:ARG:NH1	1:A:135:ARG:HG3	2.33	0.43
1:B:162:LEU:O	1:B:166:VAL:HG23	2.18	0.43
1:B:49:ALA:CB	1:B:80:PRO:HA	2.49	0.43
1:B:28:GLY:O	1:B:83:HIS:CD2	2.72	0.43
1:A:350:SER:OG	1:A:352:VAL:HG12	2.18	0.43
1:A:3:PHE:O	1:A:3:PHE:HD1	2.01	0.43
1:B:25:ASP:O	1:B:26:ASP:HB3	2.17	0.43
1:A:25:ASP:O	1:A:26:ASP:HB3	2.18	0.43
1:B:418:ASN:N	1:B:418:ASN:OD1	2.52	0.43
1:A:156:GLU:HA	1:A:198:ALA:O	2.19	0.43
1:B:353:PRO:HB2	1:B:355:GLN:HE22	1.83	0.43
1:A:253:PRO:O	1:A:254:ILE:C	2.57	0.43
1:B:236:LYS:HD3	1:B:266:TYR:CZ	2.53	0.43
1:B:347:PHE:CG	1:B:348:ASP:N	2.86	0.43
1:A:165:LEU:O	1:A:169:GLN:N	2.44	0.43
1:A:267:LEU:HD23	1:A:268:THR:CA	2.49	0.43
1:B:104:LEU:O	1:B:104:LEU:HD12	2.19	0.43
1:B:23:ILE:O	1:B:23:ILE:HG23	2.19	0.43
1:B:62:SER:N	1:B:68:LEU:HD21	2.34	0.43
1:B:68:LEU:N	1:B:68:LEU:CD2	2.81	0.43
1:A:104:LEU:HD13	1:A:105:ALA:O	2.19	0.42
1:A:343:THR:HA	1:A:371:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PHE:CD1	1:A:46:SER:N	2.87	0.42
1:B:109:ASN:C	1:B:111:THR:N	2.72	0.42
1:B:134:TYR:CE2	1:B:136:LEU:N	2.87	0.42
1:B:3:PHE:HD1	1:B:3:PHE:O	2.02	0.42
1:B:8:PHE:HB2	1:B:99:THR:CG2	2.48	0.42
1:A:129:ASN:OD1	1:A:129:ASN:C	2.57	0.42
1:A:161:ASP:O	1:A:162:LEU:C	2.58	0.42
1:A:352:VAL:HG13	1:A:352:VAL:O	2.20	0.42
1:A:69:LYS:HE2	1:A:71:ASP:OD1	2.18	0.42
1:B:115:GLY:C	1:B:117:VAL:N	2.70	0.42
1:A:267:LEU:CD2	1:A:268:THR:N	2.78	0.42
1:B:297:SER:HA	1:B:323:ASP:OD2	2.18	0.42
1:A:185:ALA:O	1:A:186:ALA:C	2.57	0.42
1:B:36:LEU:O	1:B:37:ILE:C	2.57	0.42
1:B:73:ILE:N	1:B:73:ILE:HD12	2.32	0.42
1:B:30:VAL:CG1	1:B:31:SER:H	2.32	0.42
1:B:329:LEU:HD23	1:B:329:LEU:C	2.39	0.42
1:A:48:GLY:O	1:A:81:ASN:N	2.44	0.42
1:B:185:ALA:O	1:B:186:ALA:C	2.58	0.42
1:B:267:LEU:HD12	1:B:306:ALA:HB2	2.02	0.42
1:B:107:GLU:O	1:B:119:GLY:O	2.37	0.42
1:B:186:ALA:O	1:B:187:THR:C	2.57	0.42
1:A:101:ASN:O	1:A:102:TYR:CG	2.73	0.42
1:A:215:TYR:HD2	1:A:215:TYR:C	2.22	0.42
1:B:158:PHE:CD1	1:B:158:PHE:N	2.87	0.42
1:B:175:ALA:HA	1:B:178:THR:HG23	2.02	0.42
2:B:504:LDA:H41	2:B:504:LDA:CM1	2.49	0.42
1:B:5:LEU:HB3	1:B:7:GLU:HG2	2.00	0.42
1:A:158:PHE:N	1:A:197:THR:HG22	2.35	0.42
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.84	0.42
1:B:15:ARG:CG	1:B:15:ARG:HH11	2.31	0.42
1:A:273:GLU:H	1:A:300:GLN:NE2	2.17	0.42
1:A:301:PHE:HD2	1:A:321:PHE:CD1	2.38	0.42
1:A:418:ASN:OD1	1:A:418:ASN:N	2.52	0.42
1:B:125:THR:O	1:B:125:THR:HG22	2.20	0.42
1:B:128:LEU:HB2	1:B:148:ALA:HB3	2.02	0.42
1:B:245:ARG:HB3	1:B:245:ARG:HE	1.78	0.42
1:B:346:ALA:HB3	1:B:368:TRP:CG	2.54	0.42
1:B:368:TRP:CE2	1:B:390:MET:SD	3.13	0.42
1:B:401:PRO:HD2	1:B:402:TYR:CE1	2.55	0.42
1:A:146:PHE:CZ	1:A:207:PHE:HD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ILE:CD1	2:A:503:LDA:HM21	2.50	0.41
1:B:106:THR:O	1:B:106:THR:HG22	2.19	0.41
1:B:111:THR:OG1	1:B:112:TYR:N	2.50	0.41
1:B:181:GLY:O	1:B:184:LEU:HB3	2.20	0.41
1:A:381:ALA:HB2	1:A:419:TYR:HD1	1.84	0.41
1:B:118:GLY:O	1:B:119:GLY:C	2.58	0.41
1:B:15:ARG:HD3	1:B:290:HIS:HE2	1.85	0.41
1:B:200:LEU:HB3	2:B:504:LDA:H92	2.02	0.41
1:B:267:LEU:CD2	1:B:268:THR:N	2.78	0.41
1:B:57:ASN:O	1:B:406:SER:HA	2.19	0.41
1:A:137:ASN:HD21	1:A:139:ALA:H	1.64	0.41
1:A:45:PHE:HE1	1:A:47:ALA:HB2	1.84	0.41
1:B:45:PHE:CD1	1:B:45:PHE:C	2.92	0.41
1:A:368:TRP:CE2	1:A:390:MET:SD	3.14	0.41
1:A:57:ASN:HB2	1:A:407:GLU:CG	2.47	0.41
1:B:266:TYR:CD1	1:B:266:TYR:N	2.89	0.41
1:B:367:PHE:O	1:B:390:MET:HA	2.21	0.41
1:A:378:ASN:C	1:A:380:ASP:N	2.72	0.41
1:B:353:PRO:HB2	1:B:355:GLN:OE1	2.21	0.41
1:A:158:PHE:CD2	1:A:196:LYS:HA	2.56	0.41
1:A:333:TYR:HB3	1:A:341:PHE:HB2	2.03	0.41
1:A:383:VAL:HA	1:A:416:ASN:O	2.21	0.41
1:A:420:ALA:C	1:A:421:PHE:CD2	2.90	0.41
1:B:252:LEU:HD13	1:B:254:ILE:HG23	2.02	0.41
1:B:54:PRO:HA	1:B:410:ALA:CB	2.50	0.41
1:A:111:THR:OG1	1:A:112:TYR:N	2.53	0.41
1:A:239:TYR:O	1:A:240:SER:CB	2.69	0.41
1:A:243:LEU:HD23	1:A:243:LEU:HA	1.84	0.41
1:A:110:ASP:C	1:A:110:ASP:OD2	2.58	0.41
1:A:27:ALA:HB2	1:A:44:THR:HB	2.02	0.41
1:B:267:LEU:C	1:B:267:LEU:CD2	2.84	0.41
1:B:270:ASN:N	1:B:270:ASN:ND2	2.66	0.41
1:B:304:LEU:CD2	2:B:504:LDA:HM11	2.50	0.41
1:A:24:ALA:HB2	1:A:36:LEU:HD12	2.03	0.41
1:B:161:ASP:O	1:B:162:LEU:C	2.59	0.41
1:A:15:ARG:O	1:A:16:ALA:C	2.59	0.41
1:A:200:LEU:N	1:A:200:LEU:CD1	2.82	0.41
1:A:239:TYR:OH	1:A:256:THR:O	2.29	0.41
1:B:207:PHE:N	1:B:207:PHE:CD2	2.88	0.41
1:B:307:THR:OG1	1:B:308:SER:N	2.54	0.41
1:A:153:ALA:CB	2:A:503:LDA:H81	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:O	1:A:82:MET:HB2	2.21	0.40
1:B:135:ARG:HG3	1:B:135:ARG:NH1	2.35	0.40
1:B:298:TRP:C	1:B:300:GLN:N	2.72	0.40
1:B:358:SER:C	1:B:360:SER:N	2.74	0.40
1:A:28:GLY:O	1:A:83:HIS:CD2	2.74	0.40
1:A:221:ASN:ND2	1:A:281:ASN:ND2	2.70	0.40
1:B:339:TRP:CE2	1:B:375:TYR:HD1	2.39	0.40
1:B:393:GLN:CA	1:B:393:GLN:HE21	2.33	0.40
1:A:364:GLN:NE2	1:A:408:GLY:N	2.69	0.40
1:A:54:PRO:HA	1:A:410:ALA:CB	2.51	0.40
1:B:243:LEU:HA	1:B:243:LEU:HD23	1.89	0.40
1:B:333:TYR:HB3	1:B:341:PHE:HB2	2.02	0.40
1:B:343:THR:HA	1:B:371:ALA:HA	2.03	0.40
1:A:200:LEU:HA	1:A:238:ASN:O	2.21	0.40
1:A:244:ASN:O	1:A:246:ALA:N	2.55	0.40
1:A:243:LEU:O	1:A:257:ALA:HB1	2.21	0.40
1:A:353:PRO:HB2	1:A:355:GLN:CD	2.42	0.40
1:B:175:ALA:HA	1:B:178:THR:CG2	2.51	0.40
1:B:385:VAL:HG13	1:B:414:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/427 (98%)	320 (76%)	67 (16%)	32 (8%)	1	15
1	B	419/427 (98%)	321 (77%)	65 (16%)	33 (8%)	1	15
All	All	838/854 (98%)	641 (76%)	132 (16%)	65 (8%)	1	15

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	34	GLY
1	A	38	THR
1	A	136	LEU
1	A	292	SER
1	A	297	SER
1	B	7	GLU
1	B	8	PHE
1	B	25	ASP
1	B	26	ASP
1	B	34	GLY
1	B	38	THR
1	B	136	LEU
1	B	292	SER
1	B	297	SER
1	A	25	ASP
1	A	26	ASP
1	A	119	GLY
1	A	164	GLN
1	A	174	PRO
1	A	175	ALA
1	A	283	VAL
1	A	320	GLY
1	A	400	GLY
1	B	119	GLY
1	B	164	GLN
1	B	174	PRO
1	B	175	ALA
1	B	283	VAL
1	B	320	GLY
1	B	379	LYS
1	B	400	GLY
1	A	29	ASN
1	A	82	MET
1	A	285	PRO
1	A	379	LYS
1	B	29	ASN
1	B	82	MET
1	B	240	SER
1	B	245	ARG
1	A	240	SER
1	A	245	ARG

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Mol	Chain	Res	Type
1	B	37	ILE
1	B	112	TYR
1	B	285	PRO
1	B	378	ASN
1	A	106	THR
1	A	112	TYR
1	A	247	PHE
1	B	17	TYR
1	B	78	TRP
1	B	106	THR
1	B	256	THR
1	A	37	ILE
1	A	180	GLN
1	A	254	ILE
1	B	108	PHE
1	A	28	GLY
1	B	231	VAL
1	A	166	VAL
1	B	28	GLY
1	A	253	PRO
1	B	254	ILE
1	A	231	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	329/335 (98%)	290 (88%)	39 (12%)	6	33
1	B	329/335 (98%)	290 (88%)	39 (12%)	6	33
All	All	658/670 (98%)	580 (88%)	78 (12%)	6	33

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE

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Mol	Chain	Res	Type
1	A	38	THR
1	A	42	ARG
1	A	45	PHE
1	A	72	ASN
1	A	73	ILE
1	A	84	PHE
1	A	89	ASN
1	A	99	THR
1	A	104	LEU
1	A	111	THR
1	A	134	TYR
1	A	137	ASN
1	A	138	ASN
1	A	141	SER
1	A	144	LEU
1	A	164	GLN
1	A	165	LEU
1	A	171	MET
1	A	173	SER
1	A	177	GLN
1	A	182	GLN
1	A	200	LEU
1	A	215	TYR
1	A	216	GLU
1	A	245	ARG
1	A	252	LEU
1	A	270	ASN
1	A	275	TRP
1	A	284	ASP
1	A	285	PRO
1	A	290	HIS
1	A	299	SER
1	A	304	LEU
1	A	340	THR
1	A	355	GLN
1	A	393	GLN
1	A	415	THR
1	A	418	ASN
1	B	8	PHE
1	B	38	THR
1	B	42	ARG
1	B	45	PHE

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Mol	Chain	Res	Type
1	B	72	ASN
1	B	73	ILE
1	B	80	PRO
1	B	84	PHE
1	B	89	ASN
1	B	99	THR
1	B	104	LEU
1	B	111	THR
1	B	134	TYR
1	B	137	ASN
1	B	138	ASN
1	B	141	SER
1	B	142	PHE
1	B	144	LEU
1	B	164	GLN
1	B	165	LEU
1	B	171	MET
1	B	173	SER
1	B	177	GLN
1	B	200	LEU
1	B	215	TYR
1	B	216	GLU
1	B	245	ARG
1	B	252	LEU
1	B	270	ASN
1	B	275	TRP
1	B	284	ASP
1	B	285	PRO
1	B	290	HIS
1	B	304	LEU
1	B	340	THR
1	B	355	GLN
1	B	393	GLN
1	B	415	THR
1	B	418	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	72	ASN
1	A	81	ASN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	189	ASN
1	A	194	ASN
1	A	204	GLN
1	A	248	ASN
1	A	270	ASN
1	A	281	ASN
1	A	300	GLN
1	A	302	GLN
1	A	356	ASN
1	A	393	GLN
1	A	416	ASN
1	B	29	ASN
1	B	72	ASN
1	B	81	ASN
1	B	137	ASN
1	B	204	GLN
1	B	248	ASN
1	B	270	ASN
1	B	281	ASN
1	B	300	GLN
1	B	302	GLN
1	B	316	GLN
1	B	356	ASN
1	B	393	GLN
1	B	416	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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	LDA	A	501	-	13,15,15	2.19	1 (7%)	14,17,17	2.07	4 (28%)
2	LDA	A	503	-	13,15,15	2.27	1 (7%)	14,17,17	1.79	2 (14%)
2	LDA	B	502	-	13,15,15	2.30	1 (7%)	14,17,17	1.97	4 (28%)
2	LDA	B	504	-	13,15,15	2.47	1 (7%)	14,17,17	1.92	5 (35%)

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	LDA	A	501	-	-	0/13/13/13	0/0/0/0
2	LDA	A	503	-	-	0/13/13/13	0/0/0/0
2	LDA	B	502	-	-	0/13/13/13	0/0/0/0
2	LDA	B	504	-	-	0/13/13/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	504	LDA	O1-N1	-8.72	1.25	1.42
2	B	502	LDA	O1-N1	-7.98	1.26	1.42
2	A	503	LDA	O1-N1	-7.79	1.26	1.42
2	A	501	LDA	O1-N1	-7.54	1.27	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LDA	CM2-N1-CM1	-5.08	101.28	110.99
2	A	503	LDA	CM2-N1-CM1	-4.62	102.15	110.99
2	B	502	LDA	CM2-N1-CM1	-4.16	103.02	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	LDA	CM2-N1-CM1	-3.94	103.45	110.99
2	B	502	LDA	CM1-N1-C1	-3.90	102.04	110.23
2	A	501	LDA	CM1-N1-C1	-3.74	102.37	110.23
2	B	504	LDA	CM1-N1-C1	-3.43	103.03	110.23
2	A	503	LDA	CM1-N1-C1	-2.44	105.11	110.23
2	B	504	LDA	C6-C5-C4	-2.33	102.47	114.45
2	B	504	LDA	C9-C8-C7	-2.32	102.51	114.45
2	B	502	LDA	C9-C8-C7	-2.26	102.83	114.45
2	A	501	LDA	C9-C8-C7	-2.07	103.79	114.45
2	B	504	LDA	CM2-N1-C1	2.24	114.94	110.23
2	B	502	LDA	O1-N1-C1	2.38	115.12	109.27
2	A	501	LDA	O1-N1-C1	2.47	115.33	109.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LDA	3	0
2	A	503	LDA	11	0
2	B	502	LDA	3	0
2	B	504	LDA	9	0

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	421/427 (98%)	-0.57	0 100 100	0, 8, 41, 69	0
1	B	421/427 (98%)	-0.56	0 100 100	0, 7, 38, 79	0
All	All	842/854 (98%)	-0.56	0 100 100	0, 7, 40, 79	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	LDA	B	502	16/16	0.86	0.35	5.74	8,8,8,8	0
2	LDA	A	503	16/16	0.84	0.40	4.37	8,8,8,8	0
2	LDA	B	504	16/16	0.90	0.39	3.14	8,8,8,8	0
2	LDA	A	501	16/16	0.83	0.32	2.55	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.