



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PWQ
Title : Crystal structure of Anthrax Lethal Factor complexed with Thioacetyl-Tyr-Pro-Met-Amide, a metal-chelating peptidyl small molecule inhibitor
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on : 2003-07-02
Resolution : 3.52 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

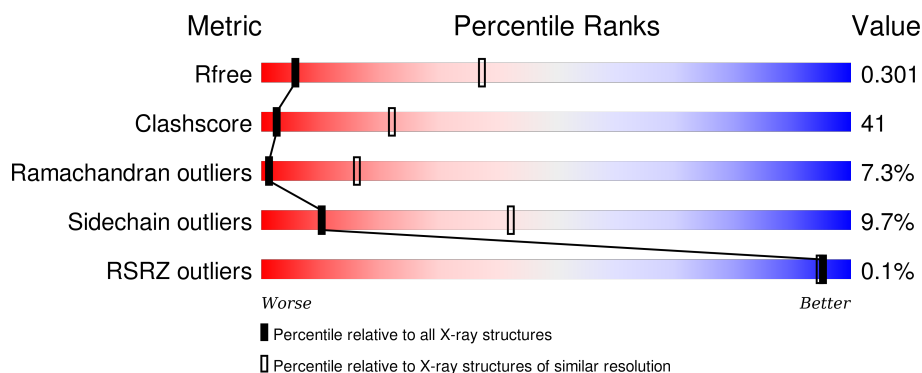
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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}	91344	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)

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	776	 31% 54% 9% 6%
1	B	776	 33% 52% 9% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12120 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.

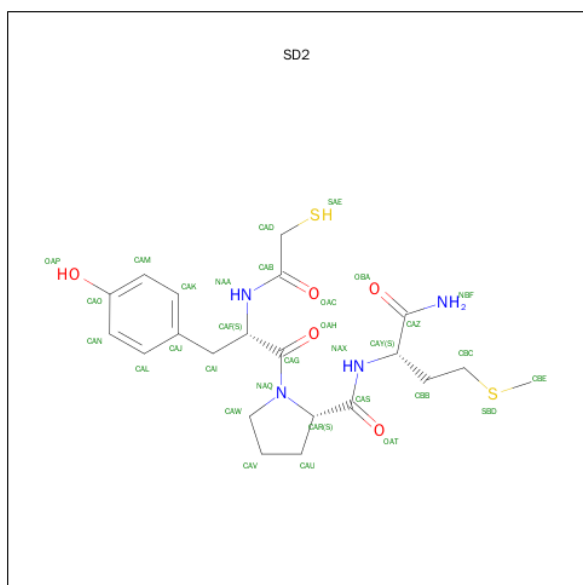
- Molecule 1 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			6020	3827	1015	1171	7			
1	B	734	Total	C	N	O	S	0	0	0
			6034	3834	1017	1176	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is N-(SULFANYLACETYL)TYROSYLPROLYLMETHIONINAMIDE (three-letter code: SD2) (formula: C₂₁H₃₀N₄O₅S₂).

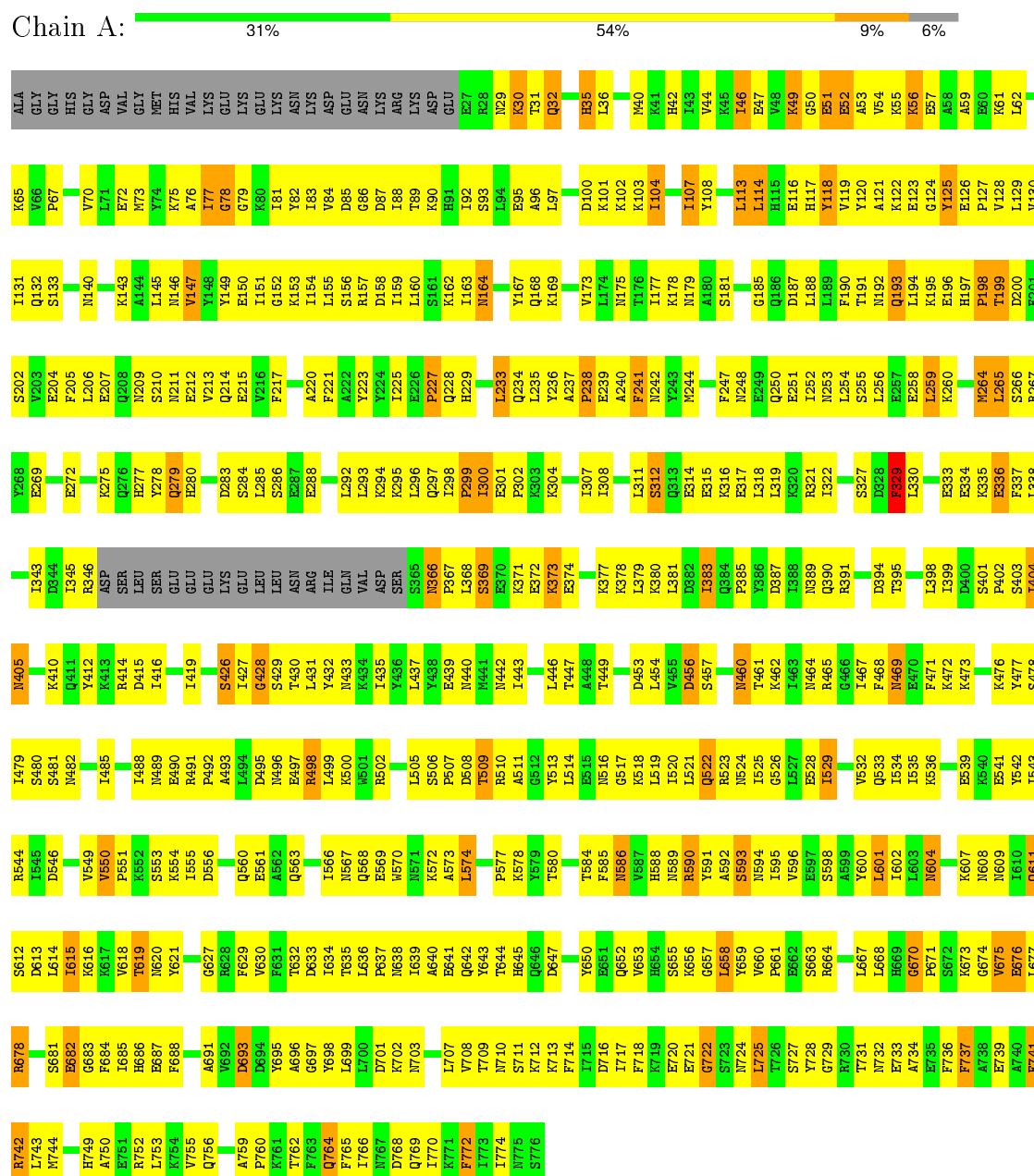


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	21	4	5	2		
3	B	1	Total	C	N	O	S	0	0
			32	21	4	5	2		

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 errors 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: Lethal factor



● Molecule 1: Lethal factor

Chain B: 33% 52% 9% 5%

ALA	GLY	GLY	HIS	HIS	ASP	VAL	GLY	GLY	ASP	ASP	GLU	E27	E28	E29	E30	E31	E32	E33	E34	E35	E36	E37	E38	E39	E40	E41	E42	E43	E44	E45	E46	E47	E48	E49	E50	E51	E52	E53	E54	E55	E56	E57	E58	E59	E60	E61	E62	E63	E64	E65	E66	E67	E68	E69	E70	E71	E72	E73	E74	E75	E76	E77	E78	E79	E80	E81	E82	E83	E84	E85	E86	E87	E88	E89	E90	E91	E92	E93	E94	E95	E96	E97	E98	E99	E100	E101	E102	E103	E104	E105	E106	E107	E108	E109	E110	E111	E112	E113	E114	E115	E116	E117	E118	E119	E120	E121	E122	E123	E124	E125	E126	E127	E128	E129	E130	E131	E132	E133	E134	E135	E136	E137	E138	E139	E140	E141	E142	E143	E144	E145	E146	E147	E148	E149	E150	E151	E152	E153	E154	E155	E156	E157	E158	E159	E160	E161	E162	E163	E164	E165	E166	E167	E168	E169	E170	E171	E172	E173	E174	E175	E176	E177	E178	E179	E180	E181	E182	E183	E184	E185	E186	E187	E188	E189	E190	E191	E192	E193	E194	E195	E196	E197	E198	E199	E200	E201	E202	E203	E204	E205	E206	E207	E208	E209	E210	E211	E212	E213	E214	E215	E216	E217	E218	E219	E220	E221	E222	E223	E224	E225	E226	E227	E228	E229	E230	E231	E232	E233	E234	E235	E236	E237	E238	E239	E240	E241	E242	E243	E244	E245	E246	E247	E248	E249	E250	E251	E252	E253	E254	E255	E256	E257	E258	E259	E260	E261	E262	E263	E264	E265	E266	E267	E268	E269	E270	E271	E272	E273	E274	E275	E276	E277	E278	E279	E280	E281	E282	E283	E284	E285	E286	E287	E288	E289	E290	E291	E292	E293	E294	E295	E296	E297	E298	E299	E300	E301	E302	E303	E304	E305	E306	E307	E308	E309	E310	E311	E312	E313	E314	E315	E316	E317	E318	E319	E320	E321	E322	E323	E324	E325	E326	E327	E328	E329	E330	E331	E332	E333	E334	E335	E336	E337	E338	E339	E340	E341	E342	E343	E344	E345	E346	E347	E348	E349	E350	E351	E352	E353	E354	E355	E356	E357	E358	E359	E360	E361	E362	E363	E364	E365	E366	E367	E368	E369	E370	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563	E564	E565	E566	E567	E568	E569	E570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	E581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	E609	E610	E611	E612	E613	E614	E615	E616	E617	E618	E619	E620	E621	E622	E623	E624	E625	E626	E627	E628	E629	E630	E631	E632	E633	E634	E635	E636	E637	E638	E639	E640	E641	E642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000	E1001	E1002	E1003	E1004	E1005	E1006	E1007	E1008	E1009	E1010	E1011	E1012	E1013	E1014	E1015	E1016	E1017	E1018	E1019	E1020	E1021	E1022	E1023	E1024	E1025	E102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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.70Å 137.40Å 98.30Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	24.86 – 3.52 24.86 – 3.51	Depositor EDS
% Data completeness (in resolution range)	86.7 (24.86-3.52) 82.4 (24.86-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.311 0.226 , 0.301	Depositor DCC
R_{free} test set	1330 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , -3.7	EDS
Estimated twinning fraction	0.066 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 31681 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12120	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SD2

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	0.48	0/6128	0.70	0/8253
1	B	0.50	0/6142	0.72	0/8272
All	All	0.49	0/12270	0.71	0/16525

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 [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	6020	0	6008	498	0
1	B	6034	0	6017	501	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	28	9	0
3	B	32	0	29	9	0
All	All	12120	0	12082	1000	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 41.

All (1000) 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:91:HIS:CD2	1:B:93:SER:HB3	1.69	1.27
1:A:635:THR:HG22	1:A:637:PRO:HD2	1.21	1.16
1:B:366:ASN:HB2	1:B:367:PRO:HD3	1.16	1.12
1:A:308:ILE:HD12	1:A:345:ILE:HD11	1.32	1.10
1:B:91:HIS:HD2	1:B:93:SER:HB3	0.92	1.09
1:B:91:HIS:CD2	1:B:93:SER:CB	2.38	1.07
1:A:49:LYS:HG3	1:A:50:GLY:H	1.24	1.02
1:B:340:LYS:O	1:B:344:ASP:OD1	1.81	0.99
1:B:366:ASN:CB	1:B:367:PRO:HD3	1.92	0.98
1:A:440:ASN:HD21	1:A:500:LYS:HE2	1.29	0.98
1:B:175:ASN:ND2	1:B:200:ASP:HB3	1.81	0.96
1:B:366:ASN:HB2	1:B:367:PRO:CD	1.89	0.96
1:B:175:ASN:HD21	1:B:200:ASP:HB3	1.28	0.95
1:B:165:GLN:HG3	1:B:166:PRO:HA	1.48	0.95
1:A:304:LYS:HD2	1:A:304:LYS:H	1.31	0.95
1:A:477:TYR:H	1:A:593:SER:HB2	1.30	0.94
1:B:296:LEU:HD22	1:B:419:ILE:HD13	1.48	0.94
1:A:426:SER:HA	1:A:510:ARG:HA	1.50	0.93
1:B:273:LYS:HD2	1:B:431:LEU:HD22	1.53	0.91
1:A:31:THR:O	1:A:35:HIS:HB3	1.70	0.91
1:A:643:TYR:HB3	1:A:652:GLN:OE1	1.72	0.90
3:B:9003:SD2:OAT	3:B:9003:SD2:HAL	1.74	0.88
1:A:500:LYS:HZ2	1:A:500:LYS:HB3	1.36	0.88
1:A:301:GLU:HG3	1:A:385:PRO:HG3	1.56	0.88
1:A:373:LYS:HG2	1:A:377:LYS:HE3	1.54	0.87
1:A:655:SER:HB2	3:A:9002:SD2:OAH	1.75	0.86
1:A:173:VAL:O	1:A:177:ILE:HG12	1.75	0.86
1:B:221:PHE:HA	1:B:244:MET:HE2	1.57	0.86
1:A:40:MET:O	1:A:44:VAL:HB	1.76	0.85
1:B:686:HIS:ND1	3:B:9003:SD2:HAK	1.92	0.85
1:A:412:TYR:O	1:A:416:ILE:HG13	1.77	0.85
1:B:516:ASN:H	1:B:516:ASN:HD22	1.23	0.84
1:B:366:ASN:HD22	1:B:367:PRO:CD	1.90	0.84
1:B:516:ASN:N	1:B:516:ASN:HD22	1.75	0.84
1:A:308:ILE:HD12	1:A:345:ILE:CD1	2.06	0.84
1:A:469:ASN:N	1:A:469:ASN:HD22	1.74	0.84
1:B:140:ASN:HD22	1:B:140:ASN:C	1.79	0.83
1:A:442:ASN:HB2	1:A:496:ASN:HD22	1.44	0.82
1:A:59:ALA:HB1	1:A:83:ILE:HD13	1.62	0.82
1:B:516:ASN:ND2	1:B:516:ASN:H	1.75	0.82
1:B:91:HIS:CD2	1:B:93:SER:H	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:PHE:CZ	1:B:534:ILE:HG13	2.16	0.81
1:B:36:LEU:HD13	1:B:64:GLU:OE1	1.80	0.81
1:A:440:ASN:ND2	1:A:500:LYS:HE2	1.96	0.81
1:A:167:TYR:CZ	1:A:536:LYS:HB2	2.16	0.80
1:A:308:ILE:CD1	1:A:345:ILE:HD11	2.11	0.80
1:A:102:LYS:HA	1:A:114:LEU:HD11	1.61	0.80
1:A:490:GLU:OE2	1:A:544:ARG:NH2	2.12	0.80
1:A:608:ASN:C	1:A:609:ASN:HD22	1.85	0.79
1:B:113:LEU:O	1:B:116:GLU:HG2	1.83	0.79
1:B:81:ILE:HG23	1:B:129:LEU:HD22	1.65	0.79
1:B:570:TRP:CE3	1:B:574:LEU:HD21	2.17	0.78
1:B:557:THR:O	1:B:561:GLU:HG3	1.82	0.78
1:B:401:SER:CB	1:B:638:ASN:HD22	1.96	0.77
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.50	0.77
1:B:186:GLN:HE21	1:B:195:LYS:HB2	1.50	0.77
1:B:75:LYS:O	1:B:78:GLY:N	2.16	0.76
1:B:611:GLN:HE21	1:B:774:ILE:CD1	1.99	0.76
1:B:304:LYS:H	1:B:304:LYS:HD3	1.47	0.76
1:B:224:TYR:HD2	1:B:225:ILE:HD13	1.51	0.76
1:A:167:TYR:CE1	1:A:536:LYS:HB2	2.21	0.76
1:B:324:ILE:O	1:B:326:SER:N	2.18	0.76
1:A:233:LEU:O	1:A:237:ALA:HB3	1.85	0.76
1:A:676:GLU:O	1:A:677:LEU:HD23	1.85	0.75
1:A:518:LYS:O	1:A:519:LEU:HD23	1.86	0.75
1:B:463:ILE:HD12	1:B:534:ILE:HG23	1.68	0.75
1:A:61:LYS:HA	1:A:61:LYS:HE2	1.69	0.75
1:A:764:GLN:O	1:A:768:ASP:HB2	1.87	0.75
1:A:73:MET:HG2	1:A:256:LEU:HD23	1.69	0.75
1:B:343:ILE:N	1:B:343:ILE:HD13	2.02	0.74
1:A:87:ASP:HB3	1:A:90:LYS:HE3	1.69	0.74
1:A:87:ASP:O	1:A:90:LYS:HG2	1.87	0.74
1:A:49:LYS:HG3	1:A:50:GLY:N	1.97	0.74
1:B:635:THR:HB	1:B:637:PRO:HD2	1.69	0.74
1:B:366:ASN:HD22	1:B:367:PRO:HD3	1.50	0.74
1:A:709:THR:HG21	1:A:734:ALA:HA	1.67	0.74
1:A:500:LYS:NZ	1:A:500:LYS:HB3	2.02	0.74
1:A:389:ASN:OD1	1:A:482:ASN:HB2	1.88	0.74
1:B:401:SER:HB2	1:B:638:ASN:HD22	1.51	0.73
1:A:658:LEU:HD23	3:A:9002:SD2:SAE	2.28	0.73
1:B:708:VAL:HG21	1:B:769:GLN:NE2	2.03	0.73
1:B:610:ILE:HD12	1:B:610:ILE:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:GLN:HE21	1:A:774:ILE:HD11	1.54	0.72
1:A:258:GLU:HG3	1:A:502:ARG:HH12	1.54	0.72
1:B:211:ASN:HA	1:B:214:GLN:NE2	2.04	0.72
1:A:613:ASP:HB3	1:A:774:ILE:HG23	1.72	0.71
1:B:145:LEU:HD23	1:B:226:GLU:HG3	1.72	0.71
1:A:677:LEU:HD11	3:A:9002:SD2:CAO	2.20	0.71
1:B:343:ILE:O	1:B:346:ARG:HB2	1.90	0.71
1:B:688:PHE:O	1:B:692:VAL:HG23	1.90	0.70
1:B:583:ILE:HG23	1:B:631:PHE:HE1	1.56	0.70
1:A:298:ILE:O	1:A:298:ILE:HD12	1.91	0.70
1:B:88:ILE:HB	1:B:130:VAL:HG11	1.73	0.70
1:B:123:GLU:HG3	1:B:157:ARG:NH1	2.06	0.70
1:A:202:SER:O	1:A:205:PHE:N	2.25	0.70
1:A:107:ILE:HG23	1:A:108:TYR:H	1.57	0.70
1:B:570:TRP:HE3	1:B:574:LEU:HD21	1.55	0.70
1:B:646:GLN:NE2	1:B:652:GLN:HB3	2.07	0.70
1:A:107:ILE:HG23	1:A:108:TYR:N	2.06	0.70
1:B:630:VAL:HB	1:B:667:LEU:HD23	1.74	0.70
1:A:95:GLU:O	1:A:95:GLU:HG3	1.91	0.70
1:B:366:ASN:CB	1:B:367:PRO:CD	2.58	0.69
1:A:567:ASN:C	1:A:569:GLU:H	1.96	0.69
1:A:113:LEU:O	1:A:117:HIS:HB2	1.91	0.69
1:B:27:GLU:O	1:B:27:GLU:HG3	1.92	0.69
1:A:693:ASP:OD2	1:A:707:LEU:HB2	1.93	0.69
1:A:500:LYS:HZ2	1:A:544:ARG:HH21	1.40	0.69
1:B:111:ASP:N	1:B:111:ASP:OD2	2.26	0.69
1:B:461:THR:HG22	1:B:540:LYS:HA	1.74	0.69
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.57	0.69
1:A:513:TYR:HA	1:A:519:LEU:CD2	2.23	0.69
1:B:70:VAL:HG13	1:B:155:LEU:HD13	1.74	0.68
1:B:278:TYR:HE2	1:B:511:ALA:O	1.76	0.68
1:B:675:VAL:HG23	3:B:9003:SD2:CAZ	2.24	0.68
1:A:513:TYR:HA	1:A:519:LEU:HD22	1.74	0.68
1:B:300:ILE:O	1:B:300:ILE:HG22	1.93	0.68
1:B:114:LEU:HA	1:B:117:HIS:HB3	1.75	0.68
1:B:233:LEU:HD23	1:B:237:ALA:HB3	1.75	0.68
1:A:395:THR:HB	1:A:398:LEU:O	1.93	0.68
1:A:442:ASN:ND2	1:A:496:ASN:HB2	2.09	0.68
1:B:107:ILE:HG21	1:B:145:LEU:HD12	1.75	0.68
1:B:246:LYS:O	1:B:250:GLN:HB2	1.94	0.68
1:B:610:ILE:CG2	1:B:614:LEU:HD23	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:SER:O	1:A:285:LEU:HD23	1.95	0.67
1:B:129:LEU:HD21	1:B:131:ILE:HG12	1.75	0.67
1:B:603:LEU:O	1:B:606:TRP:HB3	1.93	0.67
1:A:585:PHE:CE1	1:A:596:VAL:HG13	2.30	0.67
1:A:498:ARG:HD3	1:A:542:TYR:CD2	2.30	0.67
1:A:103:LYS:HG3	1:A:113:LEU:HD21	1.77	0.67
1:A:577:PRO:O	1:A:580:THR:HG22	1.95	0.67
1:A:191:THR:HG23	1:A:193:GLN:H	1.60	0.67
1:A:369:SER:OG	1:A:372:GLU:HB2	1.93	0.67
1:B:366:ASN:ND2	1:B:367:PRO:HD3	2.09	0.67
1:B:746:SER:O	1:B:752:ARG:HD2	1.94	0.67
1:B:140:ASN:HD22	1:B:141:THR:N	1.93	0.66
1:B:126:GLU:N	1:B:127:PRO:HD3	2.10	0.66
1:A:102:LYS:HA	1:A:114:LEU:CD1	2.25	0.66
1:B:516:ASN:ND2	1:B:516:ASN:N	2.40	0.66
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.30	0.66
1:B:475:PHE:CD1	1:B:529:ILE:HG12	2.30	0.66
1:B:107:ILE:O	1:B:107:ILE:HD13	1.96	0.66
1:B:643:TYR:HA	1:B:646:GLN:HB2	1.77	0.66
1:B:386:TYR:OH	1:B:411:GLN:HG3	1.95	0.66
1:B:755:VAL:HG12	1:B:763:PHE:HB2	1.78	0.66
1:A:296:LEU:HD12	1:A:419:ILE:HD13	1.78	0.65
1:B:477:TYR:H	1:B:593:SER:HB2	1.62	0.65
1:B:395:THR:HG22	1:B:638:ASN:ND2	2.11	0.65
1:A:427:ILE:HG23	1:A:428:GLY:N	2.09	0.65
1:B:438:TYR:CE2	1:B:502:ARG:HD3	2.32	0.65
1:B:212:GLU:O	1:B:216:VAL:HG23	1.96	0.65
1:A:500:LYS:HZ2	1:A:544:ARG:NH2	1.94	0.65
1:B:655:SER:HB2	3:B:9003:SD2:OAH	1.96	0.65
1:B:627:GLY:O	1:B:628:ARG:HG2	1.96	0.65
1:A:314:GLU:HA	1:A:317:GLU:CD	2.17	0.65
1:A:334:GLU:O	1:A:337:PHE:HB3	1.96	0.65
1:B:377:LYS:O	1:B:380:LYS:HB3	1.97	0.64
1:B:366:ASN:HD22	1:B:367:PRO:HD2	1.62	0.64
1:B:74:TYR:HA	1:B:159:ILE:HD11	1.79	0.64
1:A:59:ALA:CB	1:A:83:ILE:HD13	2.27	0.64
1:B:49:LYS:HG3	1:B:85:ASP:HB3	1.80	0.64
1:B:670:GLY:H	1:B:671:PRO:HD3	1.63	0.64
1:B:36:LEU:O	1:B:40:MET:HG3	1.98	0.64
1:A:304:LYS:H	1:A:304:LYS:CD	2.08	0.64
1:A:485:ILE:HG12	1:A:520:ILE:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASP:O	1:A:634:ILE:HB	1.98	0.63
1:A:427:ILE:CG2	1:A:428:GLY:N	2.61	0.63
1:A:151:ILE:O	1:A:154:ILE:HB	1.99	0.63
1:A:252:ILE:HG23	1:A:253:ASN:N	2.13	0.63
1:B:611:GLN:HE21	1:B:774:ILE:HD13	1.61	0.63
1:A:329:PHE:N	1:A:329:PHE:HD2	1.97	0.63
1:A:498:ARG:HD3	1:A:542:TYR:CE2	2.34	0.63
1:B:387:ASP:HB3	1:B:390:GLN:HB3	1.81	0.63
1:B:686:HIS:CE1	3:B:9003:SD2:HAK	2.34	0.63
1:A:673:LYS:O	3:A:9002:SD2:HAY	1.99	0.63
1:A:36:LEU:O	1:A:40:MET:HG2	1.99	0.63
1:B:45:LYS:HD2	1:B:82:TYR:CE2	2.33	0.63
1:B:650:TYR:CE1	1:B:651:GLU:HG3	2.33	0.63
1:A:73:MET:HB3	1:A:159:ILE:HD13	1.81	0.62
1:B:257:GLU:O	1:B:260:LYS:HB2	1.99	0.62
1:A:550:VAL:HG12	1:A:551:PRO:HD2	1.81	0.62
1:A:119:VAL:HG13	1:A:131:ILE:HG12	1.81	0.62
1:B:552:LYS:O	1:B:554:LYS:N	2.33	0.62
1:B:456:ASP:HB3	1:B:462:LYS:O	1.98	0.62
1:B:723:SER:HA	1:B:730:ARG:HD3	1.81	0.62
1:B:493:ALA:HB1	1:B:497:GLU:HB2	1.81	0.62
1:B:494:LEU:O	1:B:496:ASN:N	2.31	0.62
1:B:188:LEU:HD11	1:B:223:TYR:CE2	2.34	0.62
1:A:477:TYR:N	1:A:593:SER:HB2	2.10	0.62
1:A:107:ILE:C	1:A:107:ILE:HD13	2.19	0.62
1:B:232:VAL:O	1:B:235:LEU:HD12	2.00	0.62
1:A:126:GLU:O	1:A:128:VAL:HG23	1.99	0.62
1:B:366:ASN:ND2	1:B:367:PRO:CD	2.61	0.62
1:B:43:ILE:HG13	1:B:44:VAL:HG23	1.81	0.62
1:B:570:TRP:HH2	1:B:607:LYS:HB2	1.65	0.62
1:A:635:THR:HG22	1:A:637:PRO:CD	2.14	0.62
1:B:574:LEU:N	1:B:574:LEU:HD23	2.15	0.62
1:A:329:PHE:HD2	1:A:329:PHE:H	1.46	0.61
1:A:256:LEU:HD11	1:A:260:LYS:HE3	1.81	0.61
1:A:707:LEU:HD12	1:A:709:THR:CG2	2.30	0.61
1:B:105:LYS:N	1:B:105:LYS:HD2	2.15	0.61
1:B:240:ALA:O	1:B:244:MET:HB2	2.00	0.61
1:A:221:PHE:O	1:A:225:ILE:HG12	2.00	0.61
1:B:632:THR:HG21	1:B:639:ILE:HD11	1.82	0.61
1:B:650:TYR:CD1	1:B:651:GLU:HG3	2.36	0.61
1:B:503:ILE:HD13	1:B:503:ILE:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LYS:C	1:A:337:PHE:H	2.02	0.61
1:B:686:HIS:HD2	1:B:738:ALA:HB1	1.66	0.61
1:A:296:LEU:HD23	1:A:296:LEU:C	2.20	0.61
1:B:725:LEU:HD12	1:B:736:PHE:CE1	2.36	0.61
1:A:67:PRO:O	1:A:70:VAL:HG22	2.01	0.61
1:B:73:MET:HG2	1:B:256:LEU:HD12	1.83	0.61
1:B:733:GLU:CD	1:B:733:GLU:H	2.03	0.61
1:B:540:LYS:HD3	1:B:542:TYR:OH	2.00	0.61
1:A:30:LYS:HG3	1:A:30:LYS:O	1.99	0.61
1:B:242:ASN:O	1:B:243:TYR:C	2.39	0.60
1:A:102:LYS:O	1:A:114:LEU:HG	2.01	0.60
1:B:131:ILE:HD11	1:B:147:VAL:CG1	2.30	0.60
1:B:125:TYR:C	1:B:127:PRO:HD3	2.21	0.60
1:A:319:LEU:HA	1:A:322:ILE:HD12	1.81	0.60
1:B:292:LEU:HD11	1:B:418:ASN:HB3	1.82	0.60
1:B:708:VAL:HG21	1:B:769:GLN:HE22	1.67	0.60
1:B:673:LYS:HG3	1:B:673:LYS:O	2.01	0.60
1:A:635:THR:CG2	1:A:637:PRO:HD2	2.14	0.60
1:A:175:ASN:OD1	1:A:200:ASP:HB3	2.01	0.60
1:A:469:ASN:N	1:A:469:ASN:ND2	2.45	0.60
1:A:543:ILE:O	1:A:543:ILE:HG22	2.01	0.60
1:A:76:ALA:C	1:A:78:GLY:H	2.04	0.60
1:A:258:GLU:HG3	1:A:502:ARG:NH1	2.15	0.60
1:A:637:PRO:HG3	1:A:653:VAL:O	2.02	0.60
1:A:329:PHE:N	1:A:329:PHE:CD2	2.69	0.60
1:B:513:TYR:O	1:B:514:LEU:HD23	2.01	0.60
1:B:210:SER:O	1:B:212:GLU:N	2.35	0.60
1:A:191:THR:HG22	1:A:194:LEU:HG	1.83	0.60
1:B:447:THR:HG21	1:B:450:LEU:HD12	1.84	0.60
1:A:766:ILE:O	1:A:770:ILE:HG12	2.02	0.59
1:B:440:ASN:ND2	1:B:500:LYS:HD3	2.17	0.59
1:A:476:LYS:H	1:A:593:SER:CB	2.13	0.59
1:A:301:GLU:HG3	1:A:385:PRO:CG	2.30	0.59
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.82	0.59
1:A:119:VAL:HG21	1:A:147:VAL:HG22	1.85	0.59
1:B:83:ILE:HG23	1:B:131:ILE:HG22	1.83	0.59
1:B:245:ASP:C	1:B:245:ASP:OD2	2.41	0.59
1:A:338:LEU:HD21	1:A:383:ILE:HG21	1.84	0.59
1:A:608:ASN:HD22	1:A:608:ASN:N	1.99	0.59
1:B:557:THR:O	1:B:560:GLN:HG2	2.02	0.59
1:B:202:SER:O	1:B:204:GLU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:ILE:HG22	1:B:667:LEU:N	2.18	0.59
1:A:454:LEU:HA	1:A:467:ILE:HG21	1.85	0.59
1:A:330:LEU:HD21	1:A:380:LYS:HB2	1.83	0.59
1:A:739:GLU:O	1:A:743:LEU:HD12	2.03	0.59
1:B:413:LYS:O	1:B:417:GLN:HG3	2.03	0.59
1:B:636:LEU:HD12	1:B:636:LEU:N	2.16	0.58
1:A:464:ASN:OD1	1:A:467:ILE:HD13	2.03	0.58
1:B:619:THR:O	1:B:623:VAL:HG23	2.03	0.58
1:A:307:ILE:O	1:A:311:LEU:HD13	2.02	0.58
1:A:241:PHE:C	1:A:241:PHE:CD1	2.76	0.58
1:B:656:LYS:HD3	1:B:672:SER:HB3	1.83	0.58
1:A:601:LEU:HD23	1:A:601:LEU:H	1.68	0.58
1:B:221:PHE:O	1:B:225:ILE:HG12	2.04	0.58
1:B:401:SER:HB2	1:B:638:ASN:ND2	2.18	0.58
1:A:267:ARG:O	1:A:489:ASN:ND2	2.36	0.58
1:A:73:MET:CG	1:A:256:LEU:HD23	2.34	0.58
1:B:477:TYR:HB2	1:B:555:ILE:HD13	1.86	0.58
1:B:686:HIS:CD2	1:B:738:ALA:HB1	2.39	0.58
1:B:221:PHE:CD1	1:B:244:MET:HE1	2.35	0.58
1:B:202:SER:OG	1:B:204:GLU:HG3	2.03	0.58
1:A:677:LEU:HD21	3:A:9002:SD2:OAP	2.02	0.58
1:A:461:THR:O	1:A:541:GLU:HB2	2.04	0.58
1:B:155:LEU:O	1:B:159:ILE:HB	2.03	0.57
1:B:338:LEU:O	1:B:341:LEU:HB3	2.03	0.57
1:B:69:ASP:O	1:B:73:MET:HG3	2.04	0.57
1:B:496:ASN:HD22	1:B:497:GLU:N	2.02	0.57
1:A:368:LEU:O	1:A:369:SER:HB3	2.04	0.57
1:B:444:ASN:OD1	1:B:448:ALA:HA	2.04	0.57
3:A:9002:SD2:HAL	3:A:9002:SD2:OAT	2.04	0.57
1:B:224:TYR:CD2	1:B:225:ILE:HD13	2.37	0.57
1:A:338:LEU:HD22	1:A:379:LEU:HD13	1.85	0.57
1:B:571:ASN:HD21	1:B:580:THR:HG22	1.68	0.57
1:B:236:TYR:C	1:B:238:PRO:HD3	2.24	0.57
1:B:510:ARG:O	1:B:522:GLN:HB3	2.04	0.57
1:B:140:ASN:ND2	1:B:140:ASN:C	2.50	0.57
1:A:202:SER:O	1:A:205:PHE:HB3	2.04	0.57
1:B:84:VAL:O	1:B:133:SER:N	2.31	0.57
1:B:330:LEU:O	1:B:335:LYS:HE3	2.03	0.57
1:B:91:HIS:CD2	1:B:93:SER:N	2.71	0.57
1:B:555:ILE:O	1:B:558:LYS:HB2	2.05	0.57
1:B:468:PHE:CE1	1:B:534:ILE:CG1	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:THR:HG22	1:A:766:ILE:HD13	1.87	0.57
1:A:122:LYS:N	1:A:128:VAL:O	2.38	0.57
1:A:601:LEU:N	1:A:601:LEU:HD23	2.20	0.57
1:A:602:ILE:HG23	1:A:681:SER:HA	1.87	0.57
1:B:221:PHE:HD1	1:B:244:MET:CE	2.16	0.57
1:B:438:TYR:HE2	1:B:502:ARG:HD3	1.70	0.56
1:B:257:GLU:O	1:B:260:LYS:N	2.38	0.56
1:A:674:GLY:O	1:A:676:GLU:N	2.38	0.56
1:B:714:PHE:HE2	1:B:733:GLU:HB2	1.70	0.56
1:B:611:GLN:HE21	1:B:774:ILE:HD11	1.70	0.56
1:A:643:TYR:CB	1:A:652:GLN:OE1	2.48	0.56
1:B:94:LEU:O	1:B:96:ALA:N	2.38	0.56
1:B:105:LYS:HE2	1:B:111:ASP:HB3	1.87	0.56
1:B:404:ILE:HD12	1:B:408:VAL:HB	1.87	0.56
1:A:391:ARG:NH2	1:A:399:ILE:O	2.38	0.56
1:B:221:PHE:CE1	1:B:225:ILE:HD11	2.41	0.56
1:A:167:TYR:CE1	1:A:536:LYS:CB	2.88	0.56
1:B:403:SER:OG	1:B:638:ASN:ND2	2.39	0.56
1:B:583:ILE:HG23	1:B:631:PHE:CE1	2.39	0.56
1:B:438:TYR:O	1:B:486:VAL:HB	2.06	0.56
1:B:656:LYS:CD	1:B:672:SER:HB3	2.36	0.56
1:A:598:SER:O	1:A:602:ILE:HG13	2.05	0.56
1:B:131:ILE:HD11	1:B:147:VAL:HG13	1.86	0.56
1:A:737:PHE:HD2	1:A:737:PHE:C	2.09	0.56
1:B:91:HIS:CD2	1:B:93:SER:HB2	2.37	0.56
1:B:68:SER:O	1:B:71:LEU:N	2.39	0.56
1:A:737:PHE:CD2	1:A:737:PHE:C	2.80	0.55
1:A:506:SER:OG	1:A:508:ASP:HB2	2.06	0.55
1:A:658:LEU:HD22	1:A:659:TYR:N	2.21	0.55
1:A:253:ASN:O	1:A:255:SER:N	2.40	0.55
1:B:427:ILE:HG23	1:B:428:GLY:N	2.21	0.55
1:B:127:PRO:O	1:B:128:VAL:HG13	2.07	0.55
1:B:117:HIS:CG	1:B:118:TYR:H	2.24	0.55
1:A:123:GLU:HG3	1:A:123:GLU:O	2.05	0.55
1:A:639:ILE:HG21	1:A:667:LEU:CD2	2.36	0.55
1:A:681:SER:O	1:A:682:GLU:C	2.44	0.55
1:B:602:ILE:HD13	1:B:668:LEU:HD21	1.87	0.55
1:B:280:HIS:C	1:B:282:SER:H	2.10	0.55
1:B:766:ILE:C	1:B:768:ASP:H	2.10	0.55
1:A:107:ILE:CG2	1:A:108:TYR:H	2.18	0.55
1:B:713:LYS:HD2	1:B:765:PHE:HE1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ILE:HG22	1:A:526:GLY:N	2.21	0.55
1:B:35:HIS:O	1:B:39:ILE:HG12	2.06	0.55
1:B:319:LEU:HD23	1:B:345:ILE:HD11	1.89	0.55
1:A:642:GLN:OE1	1:A:653:VAL:HG22	2.07	0.55
1:A:304:LYS:HD2	1:A:304:LYS:N	2.12	0.55
1:A:477:TYR:CE1	1:A:593:SER:HA	2.40	0.55
1:B:431:LEU:O	1:B:432:TYR:HB3	2.08	0.54
1:B:714:PHE:HA	1:B:717:ILE:HG12	1.89	0.54
1:A:769:GLN:O	1:A:772:PHE:HB3	2.07	0.54
1:B:32:GLN:O	1:B:34:GLU:N	2.39	0.54
1:A:206:LEU:O	1:A:210:SER:HB3	2.07	0.54
1:B:303:LYS:HD2	1:B:305:ASP:OD1	2.06	0.54
1:A:762:THR:CG2	1:A:766:ILE:HD13	2.37	0.54
1:B:210:SER:O	1:B:211:ASN:C	2.44	0.54
1:A:122:LYS:HB3	1:A:128:VAL:HB	1.89	0.54
1:B:369:SER:OG	1:B:372:GLU:HG3	2.07	0.54
1:A:49:LYS:CG	1:A:50:GLY:N	2.69	0.54
1:A:250:GLN:HG3	1:A:251:GLU:HG2	1.90	0.54
1:A:387:ASP:HB3	1:A:390:GLN:HB3	1.90	0.54
1:B:83:ILE:HD12	1:B:131:ILE:HG21	1.88	0.54
1:A:247:PHE:CZ	1:A:252:ILE:HD12	2.42	0.54
1:B:94:LEU:HD11	1:B:130:VAL:HG21	1.90	0.54
1:B:729:GLY:O	1:B:736:PHE:HB2	2.07	0.54
1:B:275:LYS:HG3	1:B:513:TYR:CE2	2.42	0.54
1:A:749:HIS:O	1:A:752:ARG:N	2.41	0.54
1:B:635:THR:CB	1:B:637:PRO:HD2	2.37	0.54
1:A:563:GLN:HE21	1:A:584:THR:HA	1.72	0.54
1:A:156:SER:HA	1:A:160:LEU:HD12	1.89	0.54
1:A:674:GLY:HA2	3:A:9002:SD2:OAT	2.07	0.54
1:A:146:ASN:O	1:A:149:TYR:HB3	2.08	0.54
1:A:72:GLU:O	1:A:75:LYS:HB3	2.07	0.54
1:A:51:GLU:OE1	1:A:51:GLU:HA	2.08	0.54
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.36	0.54
1:A:440:ASN:ND2	1:A:493:ALA:HB2	2.23	0.54
1:B:221:PHE:CE2	1:B:225:ILE:HG13	2.42	0.54
1:A:563:GLN:O	1:A:566:ILE:HG22	2.08	0.54
1:B:280:HIS:C	1:B:282:SER:N	2.60	0.54
1:A:614:LEU:O	1:A:618:VAL:HG23	2.08	0.53
1:A:150:GLU:OE2	1:A:153:LYS:HE2	2.07	0.53
1:A:612:SER:O	1:A:616:LYS:HG3	2.08	0.53
1:B:410:LYS:O	1:B:414:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ILE:HG22	1:B:127:PRO:HG2	1.90	0.53
1:A:472:LYS:HE3	1:A:532:VAL:O	2.07	0.53
1:B:467:ILE:O	1:B:468:PHE:C	2.45	0.53
1:A:608:ASN:N	1:A:608:ASN:ND2	2.56	0.53
1:A:585:PHE:CZ	1:A:596:VAL:HG13	2.44	0.53
1:A:314:GLU:HA	1:A:317:GLU:CG	2.38	0.53
1:A:670:GLY:H	1:A:671:PRO:CD	2.20	0.53
1:A:636:LEU:C	1:A:638:ASN:H	2.11	0.53
1:A:265:LEU:O	1:A:269:GLU:HB2	2.08	0.53
1:B:468:PHE:CE1	1:B:534:ILE:HG13	2.44	0.53
1:A:314:GLU:HA	1:A:317:GLU:HG2	1.89	0.53
1:B:478:SER:O	1:B:527:LEU:HB2	2.08	0.53
1:B:636:LEU:O	1:B:637:PRO:C	2.46	0.53
1:B:468:PHE:CE1	1:B:534:ILE:HG12	2.44	0.53
1:A:167:TYR:HD2	1:A:168:GLN:H	1.57	0.53
1:A:204:GLU:O	1:A:207:GLU:HB3	2.09	0.53
1:B:737:PHE:CE1	1:B:766:ILE:HG13	2.43	0.53
1:A:677:LEU:HD11	3:A:9002:SD2:CAN	2.39	0.53
1:B:243:TYR:CD1	1:B:244:MET:N	2.77	0.53
1:B:610:ILE:N	1:B:610:ILE:HD12	2.22	0.53
1:A:190:PHE:CD1	1:A:194:LEU:HB3	2.44	0.53
1:A:210:SER:O	1:A:214:GLN:HG3	2.08	0.53
1:B:40:MET:HA	1:B:44:VAL:HG23	1.90	0.53
1:A:223:TYR:HB3	1:A:233:LEU:HD12	1.91	0.53
1:A:567:ASN:C	1:A:569:GLU:N	2.62	0.53
1:A:293:LEU:O	1:A:296:LEU:HB3	2.09	0.53
1:B:720:GLU:OE2	1:B:761:LYS:HE2	2.08	0.53
1:B:675:VAL:HG23	3:B:9003:SD2:NBF	2.23	0.53
1:B:640:ALA:HA	1:B:643:TYR:CZ	2.44	0.53
1:A:443:ILE:HD11	1:A:471:PHE:CD1	2.44	0.53
1:B:91:HIS:NE2	1:B:93:SER:HB2	2.24	0.53
1:B:243:TYR:HD1	1:B:244:MET:N	2.07	0.53
1:A:146:ASN:O	1:A:147:VAL:C	2.46	0.53
1:A:237:ALA:HB1	1:A:240:ALA:HB3	1.91	0.53
1:A:693:ASP:OD1	1:A:709:THR:HG22	2.09	0.53
1:B:77:ILE:CG2	1:B:127:PRO:HG2	2.39	0.53
1:B:448:ALA:HB3	1:B:672:SER:O	2.09	0.53
1:A:233:LEU:HD23	1:A:237:ALA:CB	2.40	0.52
1:A:253:ASN:C	1:A:255:SER:H	2.12	0.52
1:B:636:LEU:N	1:B:636:LEU:CD1	2.72	0.52
1:A:681:SER:O	1:A:684:PHE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:MET:SD	1:B:446:LEU:HD13	2.48	0.52
1:A:82:TYR:HB2	1:A:130:VAL:HG22	1.90	0.52
1:B:463:ILE:HG13	1:B:541:GLU:HB3	1.92	0.52
1:A:460:ASN:O	1:A:498:ARG:NH2	2.40	0.52
1:A:429:SER:HB3	1:A:432:TYR:CZ	2.44	0.52
1:A:437:LEU:HD12	1:A:505:LEU:HD21	1.92	0.52
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.09	0.52
1:B:614:LEU:HD13	1:B:770:ILE:HG23	1.90	0.52
1:A:278:TYR:C	1:A:280:HIS:H	2.13	0.52
1:A:286:SER:C	1:A:288:GLU:H	2.11	0.52
1:B:461:THR:O	1:B:541:GLU:HB2	2.10	0.52
1:A:155:LEU:O	1:A:160:LEU:HG	2.09	0.52
1:B:673:LYS:O	1:B:674:GLY:C	2.46	0.52
1:A:103:LYS:HG3	1:A:113:LEU:CD2	2.40	0.52
1:A:584:THR:HG21	1:A:630:VAL:HG22	1.92	0.52
1:B:46:ILE:HG22	1:B:48:VAL:HG13	1.91	0.52
1:B:570:TRP:CZ3	1:B:574:LEU:HD21	2.44	0.52
1:A:314:GLU:O	1:A:318:LEU:HG	2.09	0.52
1:A:701:ASP:O	1:A:703:ASN:N	2.42	0.52
1:A:505:LEU:HD22	1:A:505:LEU:N	2.25	0.52
1:A:253:ASN:C	1:A:255:SER:N	2.62	0.52
1:A:212:GLU:O	1:A:215:GLU:HB3	2.10	0.52
1:A:335:LYS:C	1:A:337:PHE:N	2.63	0.52
1:A:335:LYS:O	1:A:337:PHE:N	2.43	0.52
1:A:196:GLU:O	1:A:197:HIS:C	2.48	0.52
1:B:324:ILE:HG22	1:B:325:ASP:N	2.24	0.52
1:B:640:ALA:HB2	1:B:643:TYR:CZ	2.45	0.52
1:B:632:THR:OG1	1:B:633:ASP:N	2.43	0.52
1:B:319:LEU:CD2	1:B:345:ILE:HD11	2.39	0.52
1:B:732:ASN:OD1	1:B:734:ALA:N	2.43	0.52
1:B:416:ILE:O	1:B:418:ASN:N	2.42	0.52
1:B:178:LYS:HD2	1:B:201:PHE:CE1	2.44	0.52
1:B:276:GLN:NE2	1:B:431:LEU:HD11	2.25	0.51
1:A:468:PHE:HD1	1:A:543:ILE:HD11	1.75	0.51
1:A:456:ASP:OD1	1:A:464:ASN:HB2	2.10	0.51
1:A:55:LYS:HD2	1:A:133:SER:OG	2.10	0.51
1:B:174:LEU:HD22	1:B:216:VAL:HG11	1.92	0.51
1:B:640:ALA:HA	1:B:643:TYR:CE1	2.45	0.51
1:B:493:ALA:O	1:B:494:LEU:HD23	2.10	0.51
1:B:178:LYS:O	1:B:178:LYS:HG3	2.09	0.51
1:A:264:MET:O	1:A:267:ARG:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HD12	1:A:505:LEU:CD2	2.40	0.51
1:A:73:MET:CB	1:A:159:ILE:HD13	2.41	0.51
1:B:278:TYR:CE2	1:B:511:ALA:O	2.61	0.51
1:B:601:LEU:O	1:B:604:ASN:N	2.39	0.51
1:B:121:ALA:HB2	1:B:150:GLU:HG3	1.92	0.51
1:B:66:VAL:HG21	1:B:151:ILE:HD13	1.91	0.51
1:A:509:THR:OG1	1:A:549:VAL:HG11	2.11	0.51
1:B:552:LYS:C	1:B:554:LYS:H	2.14	0.51
1:A:32:GLN:O	1:A:36:LEU:HB2	2.10	0.51
1:B:592:ALA:O	1:B:593:SER:C	2.49	0.51
1:A:443:ILE:HD13	1:A:454:LEU:HD22	1.91	0.51
1:B:762:THR:HG22	1:B:766:ILE:HD13	1.91	0.51
1:B:293:LEU:O	1:B:297:GLN:HG3	2.11	0.51
1:A:374:GLU:O	1:A:377:LYS:HB2	2.11	0.51
1:A:442:ASN:HB2	1:A:496:ASN:ND2	2.22	0.51
1:B:426:SER:HA	1:B:509:THR:O	2.10	0.51
1:A:634:ILE:O	1:A:635:THR:C	2.48	0.51
1:A:500:LYS:NZ	1:A:544:ARG:NH2	2.58	0.51
1:B:463:ILE:HD11	1:B:541:GLU:C	2.32	0.51
1:A:584:THR:HG22	1:A:629:PHE:O	2.11	0.51
1:B:729:GLY:HA2	1:B:739:GLU:HG3	1.93	0.51
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.43	0.51
1:B:62:LEU:HD13	1:B:63:LEU:HD23	1.93	0.51
1:B:304:LYS:O	1:B:308:ILE:HG13	2.11	0.51
1:A:156:SER:HB3	1:A:217:PHE:HD2	1.75	0.51
1:B:520:ILE:O	1:B:520:ILE:HG23	2.11	0.51
1:A:505:LEU:CD2	1:A:505:LEU:N	2.74	0.51
1:A:83:ILE:HA	1:A:131:ILE:O	2.11	0.51
1:A:296:LEU:HD23	1:A:296:LEU:O	2.11	0.51
1:B:304:LYS:N	1:B:304:LYS:HD3	2.23	0.50
1:A:516:ASN:ND2	1:A:518:LYS:HD2	2.26	0.50
1:B:721:GLU:OE1	1:B:761:LYS:HB2	2.10	0.50
1:A:294:LYS:O	1:A:297:GLN:N	2.44	0.50
1:B:311:LEU:HD22	1:B:315:GLU:HB3	1.94	0.50
1:B:226:GLU:CD	1:B:229:HIS:HD1	2.14	0.50
1:B:660:VAL:O	1:B:664:ARG:N	2.44	0.50
1:B:269:GLU:O	1:B:273:LYS:HG2	2.12	0.50
1:A:522:GLN:HG3	1:A:523:ARG:O	2.10	0.50
1:B:300:ILE:HB	1:B:386:TYR:HB3	1.92	0.50
1:A:755:VAL:O	1:A:759:ALA:HB3	2.11	0.50
1:B:192:ASN:C	1:B:194:LEU:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HD12	1:A:505:LEU:HG	1.93	0.50
1:B:379:LEU:O	1:B:380:LYS:C	2.49	0.50
1:A:718:PHE:CD1	1:A:733:GLU:HB3	2.47	0.50
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.46	0.50
1:A:404:ILE:O	1:A:405:ASN:O	2.30	0.50
1:A:737:PHE:O	1:A:737:PHE:HD2	1.95	0.50
1:B:87:ASP:O	1:B:90:LYS:HG2	2.12	0.50
1:B:319:LEU:HD21	1:B:341:LEU:HD22	1.94	0.50
1:B:390:GLN:HA	1:B:390:GLN:NE2	2.27	0.50
1:B:713:LYS:O	1:B:717:ILE:HD11	2.12	0.50
1:A:279:GLN:O	1:A:279:GLN:HG3	2.11	0.50
1:A:87:ASP:CG	1:A:89:THR:HG1	2.14	0.49
1:B:729:GLY:CA	1:B:739:GLU:HG3	2.42	0.49
1:A:637:PRO:HB3	1:A:652:GLN:NE2	2.27	0.49
1:A:59:ALA:HB1	1:A:83:ILE:CD1	2.38	0.49
1:B:303:LYS:HD3	1:B:304:LYS:HZ1	1.76	0.49
1:B:610:ILE:HB	1:B:615:ILE:HD11	1.93	0.49
1:A:440:ASN:HD21	1:A:500:LYS:CE	2.12	0.49
1:B:125:TYR:HE2	1:B:162:LYS:HE3	1.77	0.49
1:A:30:LYS:CG	1:A:30:LYS:O	2.61	0.49
1:A:505:LEU:HD12	1:A:509:THR:HG21	1.93	0.49
1:A:658:LEU:CD2	1:A:659:TYR:N	2.76	0.49
1:A:185:GLY:HA3	1:A:236:TYR:O	2.13	0.49
3:B:9003:SD2:OAT	3:B:9003:SD2:CAL	2.54	0.49
1:A:78:GLY:O	1:A:127:PRO:HD2	2.12	0.49
1:A:298:ILE:HD12	1:A:299:PRO:O	2.12	0.49
1:B:123:GLU:HG3	1:B:157:ARG:HH11	1.76	0.49
1:B:714:PHE:CE2	1:B:733:GLU:HB2	2.47	0.49
1:A:86:GLY:O	1:A:132:GLN:NE2	2.45	0.49
1:B:83:ILE:HD12	1:B:131:ILE:CG2	2.42	0.49
1:A:202:SER:HB2	1:A:204:GLU:OE2	2.13	0.49
1:B:681:SER:O	1:B:685:ILE:HG13	2.12	0.49
1:B:40:MET:O	1:B:44:VAL:HB	2.13	0.49
1:A:252:ILE:CG2	1:A:253:ASN:N	2.76	0.49
1:A:733:GLU:HG2	1:A:734:ALA:H	1.78	0.49
1:A:152:GLY:O	1:A:153:LYS:C	2.50	0.49
1:A:153:LYS:O	1:A:157:ARG:HB3	2.13	0.49
1:A:528:GLU:OE1	1:A:550:VAL:HG21	2.13	0.49
1:B:759:ALA:N	1:B:760:PRO:HD3	2.27	0.49
1:A:177:ILE:HD12	1:A:238:PRO:HD2	1.95	0.49
1:A:314:GLU:C	1:A:317:GLU:HG2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PHE:N	1:A:244:MET:HE2	2.28	0.49
1:A:169:LYS:HE3	1:A:533:GLN:CB	2.43	0.49
1:A:572:LYS:C	1:A:574:LEU:H	2.16	0.49
1:B:91:HIS:CG	1:B:93:SER:H	2.31	0.49
1:A:508:ASP:O	1:A:509:THR:C	2.51	0.49
1:A:278:TYR:O	1:A:280:HIS:N	2.46	0.49
1:A:163:ILE:O	1:A:164:ASN:HB2	2.13	0.49
1:A:65:LYS:HE2	1:A:227:PRO:HG3	1.95	0.49
1:B:730:ARG:O	1:B:731:THR:O	2.31	0.48
1:A:443:ILE:HG13	1:A:499:LEU:HD21	1.95	0.48
1:B:194:LEU:HG	1:B:194:LEU:O	2.12	0.48
1:B:487:ASP:OD1	1:B:518:LYS:HE2	2.13	0.48
1:A:477:TYR:H	1:A:593:SER:CB	2.12	0.48
1:B:40:MET:HA	1:B:43:ILE:HG12	1.95	0.48
1:A:696:ALA:O	1:A:699:LEU:N	2.46	0.48
1:A:442:ASN:CG	1:A:496:ASN:HB2	2.34	0.48
1:B:226:GLU:OE1	1:B:229:HIS:ND1	2.36	0.48
1:A:209:ASN:O	1:A:212:GLU:HB2	2.14	0.48
1:B:718:PHE:CG	1:B:733:GLU:HB3	2.49	0.48
1:A:124:GLY:C	1:A:126:GLU:H	2.15	0.48
1:A:713:LYS:O	1:A:717:ILE:HG13	2.13	0.48
1:A:589:ASN:HB2	1:A:633:ASP:OD2	2.13	0.48
1:B:596:VAL:O	1:B:599:ALA:HB3	2.13	0.48
1:B:366:ASN:ND2	1:B:367:PRO:HD2	2.26	0.48
1:B:40:MET:C	1:B:42:HIS:H	2.17	0.48
1:B:721:GLU:HA	1:B:724:ASN:OD1	2.12	0.48
1:A:465:ARG:O	1:A:469:ASN:ND2	2.46	0.48
1:A:107:ILE:CG2	1:A:108:TYR:N	2.72	0.48
1:B:102:LYS:O	1:B:113:LEU:HD22	2.13	0.48
1:B:312:SER:O	1:B:313:GLN:C	2.51	0.48
1:B:682:GLU:HA	1:B:685:ILE:HD12	1.95	0.48
1:B:675:VAL:HG12	1:B:676:GLU:HG2	1.95	0.48
1:A:442:ASN:CB	1:A:496:ASN:HD22	2.21	0.48
1:A:76:ALA:C	1:A:78:GLY:N	2.66	0.48
1:B:229:HIS:O	1:B:232:VAL:HG23	2.13	0.48
1:B:447:THR:HG23	1:B:447:THR:O	2.13	0.48
1:A:489:ASN:O	1:A:490:GLU:C	2.51	0.48
1:A:267:ARG:HE	1:A:491:ARG:HH21	1.60	0.48
1:B:498:ARG:NH1	1:B:540:LYS:HE3	2.28	0.48
1:B:314:GLU:HG3	1:B:314:GLU:O	2.13	0.48
1:B:635:THR:HG22	1:B:654:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLU:O	1:A:317:GLU:HG2	2.14	0.48
1:B:322:ILE:HG13	1:B:372:GLU:OE2	2.14	0.48
1:B:369:SER:C	1:B:371:LYS:H	2.17	0.48
1:A:636:LEU:O	1:A:638:ASN:N	2.47	0.48
1:A:187:ASP:HA	1:A:195:LYS:HE2	1.95	0.48
1:A:733:GLU:CD	1:A:733:GLU:H	2.17	0.48
1:B:476:LYS:O	1:B:529:ILE:HB	2.14	0.48
1:B:715:ILE:O	1:B:718:PHE:HB3	2.13	0.48
1:B:65:LYS:HB3	1:B:225:ILE:HG22	1.95	0.48
1:A:741:PHE:O	1:A:744:MET:N	2.47	0.48
1:B:529:ILE:N	1:B:529:ILE:HD12	2.29	0.48
1:B:669:HIS:CE1	1:B:671:PRO:HD2	2.49	0.48
1:B:501:TRP:HB3	1:B:503:ILE:CD1	2.44	0.48
1:A:553:SER:O	1:A:554:LYS:C	2.51	0.48
1:B:72:GLU:HA	1:B:72:GLU:OE2	2.13	0.48
1:B:243:TYR:C	1:B:243:TYR:CD1	2.86	0.47
1:A:107:ILE:HG22	1:A:146:ASN:OD1	2.14	0.47
1:B:749:HIS:O	1:B:752:ARG:N	2.44	0.47
1:A:199:THR:OG1	1:A:200:ASP:N	2.47	0.47
1:A:688:PHE:O	1:A:691:ALA:HB3	2.13	0.47
1:B:636:LEU:H	1:B:636:LEU:CD1	2.27	0.47
1:B:43:ILE:HG13	1:B:44:VAL:N	2.28	0.47
1:A:256:LEU:HD13	1:A:256:LEU:C	2.34	0.47
1:A:87:ASP:OD2	1:A:89:THR:N	2.47	0.47
1:A:770:ILE:O	1:A:774:ILE:HG13	2.14	0.47
1:A:51:GLU:O	1:A:53:ALA:N	2.47	0.47
1:A:294:LYS:O	1:A:295:LYS:C	2.52	0.47
1:B:679:ASN:O	1:B:682:GLU:N	2.46	0.47
1:A:732:ASN:OD1	1:A:732:ASN:C	2.52	0.47
1:B:498:ARG:HH12	1:B:540:LYS:HG2	1.79	0.47
1:B:275:LYS:HG3	1:B:513:TYR:HE2	1.79	0.47
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.14	0.47
1:A:657:GLY:HA2	1:A:667:LEU:O	2.14	0.47
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.44	0.47
1:B:749:HIS:O	1:B:750:ALA:C	2.52	0.47
1:B:202:SER:C	1:B:204:GLU:N	2.66	0.47
1:A:286:SER:C	1:A:288:GLU:N	2.68	0.47
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.49	0.47
1:B:587:VAL:O	1:B:588:HIS:CG	2.67	0.47
1:B:530:LYS:O	1:B:531:ASP:HB2	2.14	0.47
1:A:118:TYR:OH	1:A:143:LYS:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:HIS:NE2	1:B:93:SER:CB	2.76	0.47
1:A:391:ARG:NH1	1:A:404:ILE:CD1	2.78	0.47
1:B:674:GLY:O	1:B:677:LEU:HB2	2.14	0.47
1:B:654:HIS:O	3:B:9003:SD2:HBE3	2.15	0.47
1:A:718:PHE:O	1:A:722:GLY:HA3	2.15	0.47
1:A:258:GLU:CG	1:A:502:ARG:HH12	2.25	0.47
1:B:107:ILE:HG12	1:B:149:TYR:CD1	2.49	0.47
1:B:338:LEU:HD21	1:B:379:LEU:HB3	1.96	0.47
1:A:327:SER:HB2	1:A:329:PHE:CE2	2.49	0.47
1:A:401:SER:O	1:A:403:SER:N	2.37	0.47
1:A:104:ILE:HG13	1:A:120:TYR:CE1	2.50	0.47
1:A:656:LYS:O	1:A:668:LEU:HD12	2.14	0.47
1:B:123:GLU:CG	1:B:124:GLY:H	2.28	0.47
1:A:191:THR:HG23	1:A:194:LEU:H	1.80	0.47
1:A:550:VAL:HG12	1:A:551:PRO:CD	2.43	0.47
1:A:476:LYS:N	1:A:593:SER:OG	2.34	0.47
1:B:129:LEU:HD23	1:B:129:LEU:C	2.35	0.47
1:A:693:ASP:OD2	1:A:693:ASP:O	2.33	0.47
1:A:693:ASP:CG	1:A:708:VAL:HG12	2.36	0.47
1:A:718:PHE:HA	1:A:722:GLY:HA3	1.97	0.47
1:B:511:ALA:CB	1:B:521:LEU:HA	2.45	0.47
1:B:84:VAL:HG22	1:B:85:ASP:N	2.30	0.47
1:A:725:LEU:HD12	1:A:736:PHE:CE1	2.50	0.47
1:B:564:LEU:O	1:B:568:GLN:HB2	2.15	0.47
1:A:338:LEU:CD2	1:A:383:ILE:HG21	2.45	0.47
1:A:479:ILE:HG22	1:A:480:SER:N	2.30	0.47
1:B:660:VAL:HG13	1:B:662:GLU:OE2	2.14	0.47
1:A:118:TYR:N	1:A:118:TYR:CD1	2.83	0.47
1:A:495:ASP:C	1:A:497:GLU:N	2.68	0.47
1:A:87:ASP:OD2	1:A:87:ASP:C	2.52	0.46
1:B:614:LEU:O	1:B:618:VAL:HG23	2.14	0.46
1:A:191:THR:HG21	1:A:212:GLU:OE2	2.15	0.46
1:B:280:HIS:O	1:B:282:SER:N	2.48	0.46
1:A:81:ILE:HG12	1:A:129:LEU:HD23	1.98	0.46
1:A:639:ILE:HG23	1:A:641:GLU:OE1	2.15	0.46
1:B:276:GLN:O	1:B:277:HIS:C	2.54	0.46
1:A:696:ALA:O	1:A:697:GLY:C	2.53	0.46
1:B:189:LEU:HD22	1:B:220:ALA:HB2	1.97	0.46
1:A:639:ILE:HG21	1:A:667:LEU:HD21	1.96	0.46
1:A:498:ARG:CD	1:A:542:TYR:CD2	2.97	0.46
1:B:32:GLN:C	1:B:34:GLU:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:GLY:HA3	1:B:550:VAL:O	2.16	0.46
1:A:683:GLY:O	1:A:687:GLU:HG2	2.15	0.46
1:B:472:LYS:HG3	1:B:473:LYS:N	2.29	0.46
1:A:437:LEU:HD12	1:A:505:LEU:CG	2.46	0.46
1:B:455:VAL:HG22	1:B:498:ARG:HE	1.79	0.46
1:A:718:PHE:CE1	1:A:733:GLU:N	2.84	0.46
1:A:191:THR:C	1:A:193:GLN:H	2.19	0.46
1:A:636:LEU:C	1:A:638:ASN:N	2.67	0.46
1:A:586:ASN:HB3	1:A:632:THR:OG1	2.14	0.46
1:B:261:ASP:OD1	1:B:490:GLU:HB3	2.15	0.46
1:B:366:ASN:CG	1:B:367:PRO:HD3	2.34	0.46
1:A:264:MET:O	1:A:265:LEU:C	2.54	0.46
1:B:640:ALA:C	1:B:642:GLN:N	2.69	0.46
1:A:272:GLU:HG3	1:B:125:TYR:CE1	2.51	0.46
1:B:77:ILE:HG22	1:B:77:ILE:O	2.16	0.46
1:B:331:SER:HB3	1:B:334:GLU:HB2	1.97	0.46
1:B:488:ILE:HG22	1:B:489:ASN:CG	2.36	0.46
1:A:446:LEU:HG	1:A:591:TYR:HB2	1.98	0.46
1:A:674:GLY:O	1:A:675:VAL:C	2.53	0.46
1:B:769:GLN:O	1:B:772:PHE:HB3	2.16	0.46
1:A:498:ARG:HG2	1:A:498:ARG:HH11	1.81	0.46
1:A:316:LYS:O	1:A:319:LEU:HB3	2.15	0.46
1:B:331:SER:HB3	1:B:334:GLU:CD	2.36	0.46
1:A:439:GLU:OE1	1:A:590:ARG:NH2	2.49	0.46
1:A:410:LYS:NZ	1:A:414:ARG:HH21	2.14	0.46
1:B:171:LEU:O	1:B:175:ASN:HB2	2.15	0.46
1:B:468:PHE:CG	1:B:534:ILE:HD11	2.51	0.46
1:A:54:VAL:O	1:A:57:GLU:HB3	2.16	0.46
1:A:57:GLU:O	1:A:61:LYS:N	2.36	0.46
1:B:238:PRO:O	1:B:241:PHE:HB3	2.15	0.46
1:B:247:PHE:CE2	1:B:252:ILE:HD13	2.51	0.46
1:A:311:LEU:O	1:A:312:SER:HB3	2.15	0.46
1:B:294:LYS:HG3	1:B:295:LYS:N	2.31	0.46
1:B:735:GLU:O	1:B:736:PHE:C	2.52	0.46
1:A:529:ILE:N	1:A:529:ILE:HD13	2.31	0.46
1:A:62:LEU:HD21	1:A:147:VAL:HG11	1.97	0.46
1:A:592:ALA:HA	1:A:595:ILE:HG12	1.97	0.46
1:B:636:LEU:N	1:B:637:PRO:CD	2.79	0.46
1:A:167:TYR:OH	1:A:536:LYS:HB2	2.15	0.46
1:B:376:LEU:HD23	1:B:379:LEU:HD12	1.98	0.46
1:B:557:THR:HA	1:B:560:GLN:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ALA:O	1:A:78:GLY:N	2.49	0.45
1:A:205:PHE:CE2	1:A:209:ASN:ND2	2.82	0.45
1:A:46:ILE:O	1:A:47:GLU:HG3	2.16	0.45
1:A:753:LEU:O	1:A:756:GLN:N	2.48	0.45
1:B:643:TYR:HB3	1:B:646:GLN:OE1	2.16	0.45
1:B:670:GLY:H	1:B:671:PRO:CD	2.28	0.45
1:A:481:SER:HA	1:A:524:ASN:HD22	1.80	0.45
1:A:615:ILE:HG22	1:A:616:LYS:N	2.31	0.45
1:A:427:ILE:CG2	1:A:428:GLY:H	2.30	0.45
1:A:314:GLU:CA	1:A:317:GLU:HG2	2.46	0.45
1:A:126:GLU:HG3	1:A:126:GLU:O	2.16	0.45
1:A:615:ILE:O	1:A:619:THR:HG23	2.15	0.45
1:A:695:TYR:O	1:A:698:TYR:HB3	2.17	0.45
1:B:239:GLU:O	1:B:242:ASN:N	2.49	0.45
1:A:299:PRO:O	1:A:300:ILE:HG23	2.16	0.45
1:A:191:THR:OG1	1:A:192:ASN:N	2.50	0.45
1:B:49:LYS:HB2	1:B:50:GLY:H	1.58	0.45
1:B:369:SER:O	1:B:371:LYS:N	2.49	0.45
1:A:264:MET:O	1:A:266:SER:N	2.49	0.45
1:B:467:ILE:N	1:B:467:ILE:HD12	2.32	0.45
1:A:584:THR:HG23	1:A:630:VAL:HA	1.98	0.45
1:B:731:THR:HG22	1:B:732:ASN:H	1.81	0.45
1:A:122:LYS:CB	1:A:128:VAL:HB	2.47	0.45
1:A:220:ALA:C	1:A:244:MET:HE2	2.37	0.45
1:A:682:GLU:O	1:A:685:ILE:N	2.44	0.45
1:B:487:ASP:OD2	1:B:487:ASP:N	2.49	0.45
1:A:88:ILE:HD13	1:A:118:TYR:C	2.36	0.45
1:B:74:TYR:CZ	1:B:79:GLY:HA3	2.52	0.45
1:A:429:SER:HB3	1:A:432:TYR:CE1	2.52	0.45
1:B:717:ILE:HD13	1:B:717:ILE:N	2.31	0.45
1:B:51:GLU:O	1:B:53:ALA:N	2.50	0.45
1:B:563:GLN:NE2	1:B:584:THR:HA	2.32	0.45
1:A:264:MET:HG2	1:A:265:LEU:N	2.31	0.45
1:A:191:THR:HG22	1:A:194:LEU:CG	2.47	0.45
1:B:89:THR:HG21	1:B:97:LEU:HD12	1.98	0.45
1:B:427:ILE:HG23	1:B:428:GLY:H	1.80	0.45
1:B:211:ASN:O	1:B:214:GLN:N	2.49	0.45
1:B:505:LEU:HD11	1:B:521:LEU:HD21	1.98	0.45
1:B:477:TYR:N	1:B:593:SER:HB2	2.30	0.45
1:B:264:MET:O	1:B:267:ARG:N	2.48	0.45
1:B:467:ILE:H	1:B:467:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LYS:HD3	1:B:304:LYS:NZ	2.32	0.45
1:A:73:MET:O	1:A:76:ALA:HB3	2.17	0.45
1:A:566:ILE:HG13	1:A:600:TYR:CE2	2.52	0.45
1:A:739:GLU:O	1:A:743:LEU:CD1	2.65	0.45
1:A:426:SER:HB3	1:A:508:ASP:O	2.17	0.45
1:A:61:LYS:CE	1:A:61:LYS:HA	2.45	0.45
1:A:707:LEU:HD23	1:A:707:LEU:H	1.81	0.45
1:A:611:GLN:NE2	1:A:774:ILE:HD11	2.29	0.45
1:B:587:VAL:HG11	1:B:592:ALA:HA	1.99	0.45
1:A:744:MET:SD	1:A:766:ILE:HG21	2.57	0.44
1:A:766:ILE:N	1:A:766:ILE:HD12	2.32	0.44
1:B:762:THR:C	1:B:764:GLN:N	2.70	0.44
1:A:197:HIS:HA	1:A:198:PRO:HD3	1.85	0.44
1:A:366:ASN:HB2	1:A:367:PRO:HD3	1.99	0.44
1:B:48:VAL:HB	1:B:49:LYS:H	1.51	0.44
1:A:462:LYS:HA	1:A:541:GLU:OE2	2.17	0.44
1:A:169:LYS:HE3	1:A:533:GLN:HB2	2.00	0.44
1:A:187:ASP:HA	1:A:195:LYS:CE	2.47	0.44
1:A:188:LEU:O	1:A:188:LEU:HD12	2.18	0.44
1:B:131:ILE:HD11	1:B:147:VAL:HG11	1.99	0.44
1:B:766:ILE:HG22	1:B:767:ASN:N	2.31	0.44
1:A:311:LEU:O	1:A:315:GLU:HB2	2.17	0.44
1:B:679:ASN:O	1:B:680:ASP:C	2.56	0.44
1:B:594:ASN:O	1:B:595:ILE:C	2.55	0.44
1:A:255:SER:O	1:A:256:LEU:C	2.55	0.44
1:B:155:LEU:HD12	1:B:159:ILE:CG2	2.47	0.44
1:A:427:ILE:O	1:A:428:GLY:C	2.54	0.44
1:B:721:GLU:OE2	1:B:760:PRO:N	2.51	0.44
1:A:185:GLY:CA	1:A:236:TYR:O	2.66	0.44
1:A:588:HIS:C	1:A:589:ASN:HD22	2.20	0.44
1:B:591:TYR:O	1:B:595:ILE:HG12	2.17	0.44
1:B:176:THR:O	1:B:180:ALA:N	2.46	0.44
1:B:479:ILE:O	1:B:589:ASN:C	2.56	0.44
1:B:658:LEU:HD23	1:B:659:TYR:N	2.32	0.44
1:A:639:ILE:HG21	1:A:667:LEU:HD22	2.00	0.44
1:B:640:ALA:CA	1:B:643:TYR:CZ	3.01	0.44
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.99	0.44
1:A:711:SER:OG	1:A:714:PHE:HB2	2.17	0.44
1:A:661:PRO:O	1:A:664:ARG:HG3	2.17	0.44
1:B:640:ALA:HB2	1:B:643:TYR:OH	2.17	0.44
1:B:122:LYS:HB3	1:B:128:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:NH1	1:A:404:ILE:HD13	2.33	0.44
1:A:566:ILE:O	1:A:566:ILE:HG12	2.18	0.44
1:B:693:ASP:HB2	1:B:737:PHE:CE2	2.52	0.44
1:A:371:LYS:HA	1:A:371:LYS:HD2	1.81	0.44
1:A:31:THR:HG22	1:A:32:GLN:N	2.32	0.44
1:B:466:GLY:O	1:B:467:ILE:C	2.56	0.44
1:A:765:PHE:O	1:A:768:ASP:HB3	2.17	0.44
1:A:523:ARG:O	1:A:524:ASN:HB2	2.17	0.44
1:B:758:ASN:C	1:B:760:PRO:HD3	2.37	0.44
1:B:113:LEU:HB2	1:B:116:GLU:OE1	2.18	0.44
1:B:511:ALA:HB2	1:B:521:LEU:HA	2.00	0.44
1:A:506:SER:O	1:A:507:PRO:C	2.56	0.44
1:B:505:LEU:HD23	1:B:549:VAL:HG21	1.99	0.44
1:A:600:TYR:O	1:A:604:ASN:HB2	2.17	0.44
1:B:670:GLY:N	1:B:671:PRO:CD	2.81	0.44
1:B:765:PHE:O	1:B:768:ASP:HB3	2.18	0.44
1:B:222:ALA:O	1:B:223:TYR:C	2.56	0.44
1:B:416:ILE:C	1:B:418:ASN:N	2.71	0.44
1:A:378:LYS:HG2	1:A:650:TYR:CD2	2.53	0.44
1:A:488:ILE:HG13	1:A:517:GLY:O	2.18	0.44
1:A:440:ASN:CG	1:A:493:ALA:HB2	2.38	0.43
1:A:660:VAL:HA	1:A:661:PRO:HD3	1.91	0.43
1:B:503:ILE:CD1	1:B:503:ILE:N	2.78	0.43
1:A:241:PHE:HD1	1:A:241:PHE:C	2.20	0.43
1:A:522:GLN:HG2	1:A:525:ILE:HD11	1.99	0.43
1:A:335:LYS:CG	1:A:336:GLU:N	2.81	0.43
1:B:766:ILE:C	1:B:768:ASP:N	2.71	0.43
1:B:490:GLU:HG3	1:B:491:ARG:N	2.33	0.43
1:B:89:THR:O	1:B:89:THR:HG22	2.18	0.43
1:B:193:GLN:HB3	1:B:193:GLN:HE21	1.61	0.43
1:A:500:LYS:HB3	1:A:544:ARG:HH21	1.83	0.43
1:A:614:LEU:HD22	1:A:770:ILE:HD12	2.00	0.43
1:B:640:ALA:C	1:B:642:GLN:H	2.20	0.43
1:B:412:TYR:O	1:B:416:ILE:HG12	2.18	0.43
1:A:84:VAL:O	1:A:133:SER:N	2.51	0.43
1:A:345:ILE:HG22	1:A:345:ILE:O	2.18	0.43
1:B:468:PHE:O	1:B:471:PHE:HB3	2.18	0.43
1:B:84:VAL:C	1:B:133:SER:HB3	2.37	0.43
1:A:154:ILE:HA	1:A:158:ASP:OD1	2.19	0.43
1:A:145:LEU:HD22	1:A:229:HIS:NE2	2.33	0.43
1:B:415:ASP:O	1:B:419:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:PHE:O	1:A:742:ARG:C	2.57	0.43
1:A:634:ILE:HG13	1:A:635:THR:O	2.18	0.43
1:A:640:ALA:HA	1:A:643:TYR:CZ	2.53	0.43
1:A:435:ILE:HG22	1:A:437:LEU:HG	2.01	0.43
1:B:83:ILE:HG23	1:B:131:ILE:CG2	2.47	0.43
1:B:155:LEU:HD12	1:B:159:ILE:HB	2.01	0.43
1:B:297:GLN:OE1	1:B:514:LEU:HD13	2.19	0.43
1:A:479:ILE:CG2	1:A:480:SER:N	2.82	0.43
1:A:714:PHE:O	1:A:717:ILE:N	2.39	0.43
1:B:309:HIS:O	1:B:310:SER:HB3	2.18	0.43
1:B:239:GLU:O	1:B:240:ALA:C	2.56	0.43
1:A:79:GLY:HA3	1:A:127:PRO:HB2	1.99	0.43
1:B:610:ILE:HG21	1:B:614:LEU:HD23	1.98	0.43
1:B:79:GLY:HA2	1:B:127:PRO:HB2	2.00	0.43
1:B:476:LYS:N	1:B:593:SER:OG	2.42	0.43
1:B:379:LEU:O	1:B:382:ASP:N	2.51	0.43
1:B:690:HIS:CE1	1:B:735:GLU:OE1	2.72	0.43
1:B:388:ILE:HG23	1:B:416:ILE:HD11	2.00	0.43
1:B:679:ASN:C	1:B:681:SER:N	2.72	0.43
1:A:534:ILE:HG22	1:A:535:ILE:N	2.33	0.43
1:A:56:LYS:HG3	1:A:56:LYS:O	2.18	0.43
1:B:125:TYR:CE2	1:B:162:LYS:HE3	2.53	0.43
1:A:429:SER:OG	1:A:430:THR:N	2.52	0.43
1:A:155:LEU:HG	1:A:160:LEU:HD11	2.00	0.43
1:B:257:GLU:O	1:B:258:GLU:C	2.54	0.43
1:A:234:GLN:HG3	1:A:241:PHE:CD2	2.53	0.43
1:A:525:ILE:CG2	1:A:526:GLY:N	2.82	0.43
1:A:140:ASN:HD21	1:A:143:LYS:NZ	2.16	0.43
1:A:640:ALA:HA	1:A:643:TYR:CE2	2.54	0.43
1:A:107:ILE:C	1:A:107:ILE:CD1	2.87	0.43
1:B:639:ILE:O	1:B:642:GLN:N	2.44	0.43
1:B:766:ILE:O	1:B:768:ASP:N	2.52	0.43
1:A:621:TYR:CE1	1:A:664:ARG:CZ	3.02	0.42
1:B:202:SER:O	1:B:205:PHE:N	2.51	0.42
1:B:65:LYS:HA	1:B:65:LYS:HD2	1.81	0.42
1:B:117:HIS:CG	1:B:118:TYR:N	2.87	0.42
1:A:480:SER:HB3	1:A:525:ILE:HB	2.00	0.42
1:A:29:ASN:C	1:A:31:THR:H	2.21	0.42
1:A:32:GLN:O	1:A:36:LEU:CB	2.68	0.42
1:A:611:GLN:HE22	1:A:770:ILE:CG2	2.32	0.42
1:B:718:PHE:HZ	1:B:731:THR:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ASN:C	1:B:496:ASN:HD22	2.21	0.42
1:B:610:ILE:CD1	1:B:610:ILE:H	2.27	0.42
1:A:415:ASP:O	1:A:419:ILE:HG13	2.19	0.42
1:B:713:LYS:HD2	1:B:765:PHE:CE1	2.53	0.42
1:B:737:PHE:O	1:B:740:ALA:HB3	2.19	0.42
1:A:221:PHE:CE1	1:A:225:ILE:HD11	2.54	0.42
1:A:206:LEU:CD1	1:A:213:VAL:HG11	2.49	0.42
1:A:555:ILE:HD12	1:A:555:ILE:N	2.34	0.42
1:B:388:ILE:O	1:B:391:ARG:N	2.47	0.42
1:A:467:ILE:H	1:A:467:ILE:CD1	2.33	0.42
1:B:264:MET:C	1:B:266:SER:N	2.73	0.42
1:B:436:TYR:CE2	1:B:504:GLN:HB2	2.54	0.42
1:A:707:LEU:N	1:A:707:LEU:HD23	2.34	0.42
1:B:237:ALA:N	1:B:238:PRO:HD3	2.35	0.42
1:A:190:PHE:HD1	1:A:194:LEU:HB3	1.84	0.42
1:B:319:LEU:HD23	1:B:345:ILE:CD1	2.49	0.42
1:A:311:LEU:O	1:A:312:SER:CB	2.67	0.42
1:B:60:GLU:O	1:B:62:LEU:N	2.52	0.42
1:A:570:TRP:HH2	1:A:607:LYS:HB2	1.85	0.42
1:A:77:ILE:CG2	1:A:162:LYS:HD2	2.50	0.42
1:B:654:HIS:O	3:B:9003:SD2:CBE	2.68	0.42
1:B:70:VAL:HG22	1:B:252:ILE:HD11	2.02	0.42
1:B:437:LEU:HD11	1:B:519:LEU:HD12	2.02	0.42
1:A:645:HIS:NE2	1:A:663:SER:HB3	2.34	0.42
1:B:56:LYS:C	1:B:58:ALA:N	2.73	0.42
1:A:686:HIS:C	1:A:686:HIS:CD2	2.93	0.42
1:A:469:ASN:H	1:A:469:ASN:ND2	2.15	0.42
1:A:159:ILE:HG23	1:A:259:LEU:HD11	2.01	0.42
1:B:416:ILE:HG22	1:B:420:ASP:OD1	2.20	0.42
1:B:60:GLU:C	1:B:62:LEU:N	2.72	0.42
1:A:725:LEU:HB2	1:A:736:PHE:HE1	1.83	0.42
1:A:366:ASN:H	1:A:367:PRO:CD	2.32	0.42
1:B:30:LYS:HG3	1:B:30:LYS:O	2.20	0.42
1:B:427:ILE:O	1:B:432:TYR:OH	2.35	0.42
1:A:70:VAL:HG12	1:A:252:ILE:HD11	2.01	0.42
1:A:693:ASP:C	1:A:693:ASP:OD2	2.58	0.42
1:B:657:GLY:HA2	1:B:667:LEU:O	2.20	0.42
1:A:403:SER:HB2	1:A:638:ASN:OD1	2.20	0.42
1:A:563:GLN:HE21	1:A:585:PHE:H	1.68	0.42
1:B:313:GLN:C	1:B:315:GLU:H	2.22	0.42
1:B:190:PHE:CB	1:B:194:LEU:HD23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:TYR:CE2	1:B:661:PRO:HG3	2.55	0.42
1:B:578:LYS:O	1:B:579:TYR:HB2	2.20	0.42
1:B:498:ARG:HA	1:B:498:ARG:HD2	1.92	0.41
1:B:303:LYS:CD	1:B:304:LYS:HZ1	2.33	0.41
1:B:77:ILE:CG2	1:B:77:ILE:O	2.68	0.41
1:B:732:ASN:OD1	1:B:734:ALA:HB3	2.20	0.41
1:B:324:ILE:O	1:B:325:ASP:C	2.59	0.41
1:B:234:GLN:HB2	1:B:241:PHE:CD2	2.55	0.41
1:B:264:MET:O	1:B:266:SER:N	2.53	0.41
1:A:125:TYR:HA	1:B:268:TYR:HE2	1.86	0.41
1:A:560:GLN:O	1:A:561:GLU:C	2.59	0.41
1:A:96:ALA:O	1:A:97:LEU:C	2.59	0.41
1:A:567:ASN:O	1:A:569:GLU:N	2.49	0.41
1:B:529:ILE:N	1:B:529:ILE:CD1	2.83	0.41
1:B:45:LYS:HD2	1:B:82:TYR:HE2	1.80	0.41
1:B:619:THR:O	1:B:619:THR:HG22	2.19	0.41
1:B:206:LEU:HD23	1:B:213:VAL:HG21	2.03	0.41
1:A:394:ASP:HB3	1:A:635:THR:OG1	2.20	0.41
1:A:655:SER:HA	3:A:9002:SD2:CBE	2.51	0.41
1:A:618:VAL:O	1:A:621:TYR:HB3	2.20	0.41
1:A:369:SER:OG	1:A:372:GLU:CB	2.67	0.41
1:B:388:ILE:HG23	1:B:416:ILE:CD1	2.50	0.41
1:A:228:GLN:OE1	1:A:228:GLN:HA	2.19	0.41
1:A:733:GLU:HG2	1:A:734:ALA:N	2.35	0.41
1:B:420:ASP:CG	1:B:523:ARG:HH11	2.24	0.41
1:A:178:LYS:HG3	1:A:179:ASN:ND2	2.34	0.41
1:A:118:TYR:CE2	1:A:143:LYS:HB3	2.56	0.41
1:B:467:ILE:H	1:B:467:ILE:CD1	2.33	0.41
1:A:114:LEU:C	1:A:116:GLU:H	2.24	0.41
1:A:608:ASN:C	1:A:609:ASN:ND2	2.64	0.41
1:B:610:ILE:HG23	1:B:614:LEU:HD23	1.99	0.41
1:B:174:LEU:CD2	1:B:216:VAL:HG11	2.51	0.41
1:A:272:GLU:HA	1:A:275:LYS:HB3	2.01	0.41
1:B:114:LEU:HD22	1:B:120:TYR:HB2	2.01	0.41
1:A:175:ASN:O	1:A:178:LYS:HG2	2.21	0.41
1:B:468:PHE:CD2	1:B:534:ILE:HD11	2.56	0.41
1:B:401:SER:CB	1:B:638:ASN:ND2	2.75	0.41
1:A:247:PHE:CG	1:A:247:PHE:O	2.73	0.41
1:B:74:TYR:CE1	1:B:79:GLY:HA3	2.55	0.41
1:B:294:LYS:C	1:B:296:LEU:H	2.22	0.41
1:A:301:GLU:HA	1:A:302:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:LYS:HD3	1:B:542:TYR:CZ	2.55	0.41
1:A:563:GLN:NE2	1:A:585:PHE:H	2.17	0.41
1:B:755:VAL:HG12	1:B:756:GLN:N	2.34	0.41
1:B:257:GLU:HA	1:B:260:LYS:HD3	2.03	0.41
1:A:319:LEU:HD13	1:A:319:LEU:C	2.41	0.41
1:A:311:LEU:O	1:A:315:GLU:OE1	2.39	0.41
1:A:721:GLU:OE1	1:A:759:ALA:HA	2.20	0.41
1:A:235:LEU:HD23	1:A:236:TYR:CE2	2.56	0.41
1:A:121:ALA:HA	1:A:129:LEU:HA	2.02	0.41
1:B:473:LYS:O	1:B:474:ASN:HB2	2.20	0.41
1:B:743:LEU:O	1:B:744:MET:C	2.59	0.41
1:A:677:LEU:O	1:A:678:ARG:C	2.59	0.41
1:B:143:LYS:O	1:B:147:VAL:HG23	2.21	0.41
1:B:186:GLN:NE2	1:B:195:LYS:HB2	2.25	0.41
1:B:27:GLU:CG	1:B:27:GLU:O	2.63	0.41
1:A:391:ARG:CZ	1:A:395:THR:HG21	2.51	0.41
1:A:430:THR:O	1:A:431:LEU:HD23	2.21	0.41
1:A:427:ILE:HA	1:A:427:ILE:HD12	1.81	0.41
1:A:151:ILE:O	1:A:152:GLY:C	2.57	0.41
1:A:241:PHE:HD1	1:A:242:ASN:N	2.18	0.41
1:A:169:LYS:HE3	1:A:533:GLN:HB3	2.03	0.41
1:A:118:TYR:HE2	1:A:143:LYS:HB3	1.86	0.41
1:B:490:GLU:HG2	1:B:537:GLN:HE22	1.86	0.41
1:A:728:TYR:O	1:A:729:GLY:C	2.59	0.41
1:B:235:LEU:HD13	1:B:236:TYR:CD1	2.56	0.41
1:B:341:LEU:O	1:B:341:LEU:HD23	2.21	0.41
1:A:154:ILE:HG22	1:A:155:LEU:N	2.35	0.41
1:B:673:LYS:CG	1:B:673:LYS:O	2.68	0.41
1:A:522:GLN:HG3	1:A:523:ARG:N	2.36	0.41
1:B:113:LEU:H	1:B:116:GLU:CD	2.25	0.40
1:A:223:TYR:HB3	1:A:233:LEU:CD1	2.50	0.40
1:B:408:VAL:O	1:B:411:GLN:HB3	2.21	0.40
1:A:634:ILE:HD11	1:A:639:ILE:HD12	2.02	0.40
1:A:73:MET:SD	1:A:159:ILE:HG21	2.61	0.40
1:B:343:ILE:HG23	1:B:346:ARG:HD2	2.01	0.40
1:A:681:SER:O	1:A:684:PHE:HB3	2.21	0.40
1:A:511:ALA:HB2	1:A:521:LEU:HD23	2.03	0.40
1:B:106:ASP:OD2	1:B:110:LYS:HB2	2.21	0.40
1:B:234:GLN:HB2	1:B:241:PHE:CE2	2.57	0.40
1:A:467:ILE:N	1:A:467:ILE:HD12	2.36	0.40
1:A:478:SER:OG	1:A:590:ARG:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:THR:HG21	1:B:97:LEU:CD1	2.52	0.40
1:A:640:ALA:O	1:A:644:THR:HG23	2.22	0.40
1:B:177:ILE:CG2	1:B:186:GLN:HA	2.51	0.40
1:B:303:LYS:NZ	1:B:304:LYS:HZ1	2.18	0.40
1:B:226:GLU:HA	1:B:227:PRO:HD3	1.94	0.40
1:B:256:LEU:O	1:B:257:GLU:C	2.59	0.40
1:A:749:HIS:O	1:A:750:ALA:C	2.60	0.40
1:A:266:SER:O	1:A:269:GLU:HB3	2.22	0.40
1:B:511:ALA:CB	1:B:521:LEU:HD23	2.51	0.40
1:B:510:ARG:HB2	1:B:522:GLN:OE1	2.22	0.40
1:B:202:SER:O	1:B:203:VAL:C	2.60	0.40
1:B:202:SER:C	1:B:204:GLU:H	2.25	0.40
1:B:322:ILE:O	1:B:342:GLN:NE2	2.53	0.40
1:A:278:TYR:C	1:A:280:HIS:N	2.75	0.40
1:A:721:GLU:HA	1:A:724:ASN:OD1	2.22	0.40
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.81	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	728/776 (94%)	529 (73%)	144 (20%)	55 (8%)	1	14
1	B	730/776 (94%)	536 (73%)	143 (20%)	51 (7%)	1	17
All	All	1458/1552 (94%)	1065 (73%)	287 (20%)	106 (7%)	1	16

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	92	ILE

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Mol	Chain	Res	Type
1	A	227	PRO
1	A	238	PRO
1	A	405	ASN
1	A	457	SER
1	A	473	LYS
1	A	539	GLU
1	A	675	VAL
1	A	678	ARG
1	A	702	LYS
1	A	720	GLU
1	B	33	GLU
1	B	95	GLU
1	B	211	ASN
1	B	310	SER
1	B	325	ASP
1	B	366	ASN
1	B	495	ASP
1	B	553	SER
1	B	731	THR
1	A	181	SER
1	A	279	GLN
1	A	336	GLU
1	A	369	SER
1	A	428	GLY
1	A	573	ALA
1	A	590	ARG
1	A	615	ILE
1	A	647	ASP
1	A	676	GLU
1	B	35	HIS
1	B	96	ALA
1	B	157	ARG
1	B	168	GLN
1	B	203	VAL
1	B	210	SER
1	B	242	ASN
1	B	250	GLN
1	B	324	ILE
1	B	326	SER
1	B	367	PRO
1	B	370	GLU
1	B	417	GLN

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Mol	Chain	Res	Type
1	B	515	GLU
1	B	592	ALA
1	B	593	SER
1	A	30	LYS
1	A	125	TYR
1	A	254	LEU
1	A	265	LEU
1	A	312	SER
1	A	460	ASN
1	A	509	THR
1	A	568	GLN
1	A	593	SER
1	A	741	PHE
1	A	760	PRO
1	B	48	VAL
1	B	52	GLU
1	B	123	GLU
1	B	187	ASP
1	B	531	ASP
1	B	767	ASN
1	A	114	LEU
1	A	198	PRO
1	A	264	MET
1	A	299	PRO
1	A	300	ILE
1	A	329	PHE
1	A	492	PRO
1	A	682	GLU
1	B	53	ALA
1	B	180	ALA
1	B	200	ASP
1	B	468	PHE
1	B	474	ASN
1	B	666	ILE
1	B	732	ASN
1	A	77	ILE
1	A	164	ASN
1	A	402	PRO
1	A	731	THR
1	A	742	ARG
1	B	142	GLU
1	B	169	LYS

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Mol	Chain	Res	Type
1	B	265	LEU
1	B	314	GLU
1	B	464	ASN
1	B	647	ASP
1	A	78	GLY
1	A	433	ASN
1	A	670	GLY
1	B	674	GLY
1	A	529	ILE
1	A	627	GLY
1	A	722	GLY
1	B	198	PRO
1	B	227	PRO
1	A	147	VAL
1	A	366	ASN
1	A	383	ILE
1	B	466	GLY
1	B	467	ILE
1	B	595	ILE
1	B	383	ILE

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	671/710 (94%)	607 (90%)	64 (10%)	11	43
1	B	673/710 (95%)	607 (90%)	66 (10%)	10	42
All	All	1344/1420 (95%)	1214 (90%)	130 (10%)	10	42

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	35	HIS
1	A	42	HIS

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Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	LYS
1	A	51	GLU
1	A	52	GLU
1	A	56	LYS
1	A	85	ASP
1	A	93	SER
1	A	100	ASP
1	A	101	LYS
1	A	104	ILE
1	A	107	ILE
1	A	113	LEU
1	A	118	TYR
1	A	193	GLN
1	A	199	THR
1	A	211	ASN
1	A	233	LEU
1	A	239	GLU
1	A	241	PHE
1	A	259	LEU
1	A	283	ASP
1	A	292	LEU
1	A	321	ARG
1	A	329	PHE
1	A	333	GLU
1	A	343	ILE
1	A	346	ARG
1	A	373	LYS
1	A	381	LEU
1	A	404	ILE
1	A	426	SER
1	A	447	THR
1	A	449	THR
1	A	453	ASP
1	A	456	ASP
1	A	469	ASN
1	A	498	ARG
1	A	514	LEU
1	A	522	GLN
1	A	546	ASP
1	A	550	VAL
1	A	556	ASP

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Mol	Chain	Res	Type
1	A	574	LEU
1	A	578	LYS
1	A	586	ASN
1	A	594	ASN
1	A	601	LEU
1	A	604	ASN
1	A	611	GLN
1	A	619	THR
1	A	620	ASN
1	A	658	LEU
1	A	693	ASP
1	A	710	ASN
1	A	712	LYS
1	A	716	ASP
1	A	725	LEU
1	A	727	SER
1	A	737	PHE
1	A	764	GLN
1	A	772	PHE
1	B	28	ARG
1	B	32	GLN
1	B	36	LEU
1	B	60	GLU
1	B	62	LEU
1	B	92	ILE
1	B	105	LYS
1	B	107	ILE
1	B	111	ASP
1	B	128	VAL
1	B	131	ILE
1	B	136	ASP
1	B	140	ASN
1	B	178	LYS
1	B	193	GLN
1	B	197	HIS
1	B	199	THR
1	B	203	VAL
1	B	204	GLU
1	B	206	LEU
1	B	209	ASN
1	B	228	GLN
1	B	233	LEU

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Mol	Chain	Res	Type
1	B	235	LEU
1	B	242	ASN
1	B	250	GLN
1	B	282	SER
1	B	296	LEU
1	B	297	GLN
1	B	304	LYS
1	B	309	HIS
1	B	323	GLN
1	B	343	ILE
1	B	344	ASP
1	B	346	ARG
1	B	366	ASN
1	B	381	LEU
1	B	384	GLN
1	B	398	LEU
1	B	407	ASP
1	B	408	VAL
1	B	433	ASN
1	B	445	ASN
1	B	449	THR
1	B	456	ASP
1	B	464	ASN
1	B	475	PHE
1	B	487	ASP
1	B	496	ASN
1	B	503	ILE
1	B	516	ASN
1	B	523	ARG
1	B	533	GLN
1	B	556	ASP
1	B	571	ASN
1	B	580	THR
1	B	586	ASN
1	B	611	GLN
1	B	613	ASP
1	B	620	ASN
1	B	647	ASP
1	B	652	GLN
1	B	712	LYS
1	B	733	GLU
1	B	747	THR

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Mol	Chain	Res	Type
1	B	753	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	32	GLN
1	A	132	GLN
1	A	140	ASN
1	A	164	ASN
1	A	179	ASN
1	A	186	GLN
1	A	193	GLN
1	A	197	HIS
1	A	214	GLN
1	A	276	GLN
1	A	323	GLN
1	A	440	ASN
1	A	444	ASN
1	A	460	ASN
1	A	469	ASN
1	A	496	ASN
1	A	504	GLN
1	A	524	ASN
1	A	563	GLN
1	A	571	ASN
1	A	589	ASN
1	A	608	ASN
1	A	609	ASN
1	A	611	GLN
1	A	620	ASN
1	A	710	ASN
1	B	91	HIS
1	B	140	ASN
1	B	165	GLN
1	B	186	GLN
1	B	193	GLN
1	B	214	GLN
1	B	228	GLN
1	B	234	GLN
1	B	242	ASN
1	B	276	GLN

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Mol	Chain	Res	Type
1	B	277	HIS
1	B	342	GLN
1	B	366	ASN
1	B	390	GLN
1	B	440	ASN
1	B	445	ASN
1	B	496	ASN
1	B	516	ASN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	571	ASN
1	B	589	ASN
1	B	609	ASN
1	B	611	GLN
1	B	620	ASN
1	B	638	ASN
1	B	645	HIS
1	B	710	ASN
1	B	756	GLN
1	B	764	GLN
1	B	769	GLN

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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	SD2	A	9002	2	33,33,33	0.93	1 (3%)	44,44,44	1.84	5 (11%)
3	SD2	B	9003	2	33,33,33	1.10	3 (9%)	44,44,44	2.19	7 (15%)

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	SD2	A	9002	2	-	0/32/44/44	0/2/2/2
3	SD2	B	9003	2	-	0/32/44/44	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9002	SD2	CBB-CBC	-3.32	1.37	1.51
3	B	9003	SD2	CBB-CBC	-3.13	1.38	1.51
3	B	9003	SD2	CBB-CAY	-2.02	1.48	1.53
3	B	9003	SD2	CAR-NAQ	2.22	1.51	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	9002	SD2	CBB-CAY-NAX	-5.77	99.87	110.87
3	A	9002	SD2	CAR-CAS-NAX	-4.54	106.44	116.64
3	B	9003	SD2	OAT-CAS-NAX	-3.85	115.39	122.93
3	B	9003	SD2	CAS-CAR-NAQ	-2.82	105.42	112.59
3	B	9003	SD2	CBE-SBD-CBC	2.12	107.61	100.37
3	B	9003	SD2	CBB-CAY-CAZ	2.21	115.67	110.32
3	A	9002	SD2	CBC-CBB-CAY	2.27	119.87	113.02
3	A	9002	SD2	OAT-CAS-NAX	3.86	130.48	122.93
3	B	9003	SD2	CBB-CAY-NAX	4.99	120.38	110.87
3	B	9003	SD2	CAR-CAS-NAX	5.32	128.60	116.64
3	A	9002	SD2	CAY-NAX-CAS	7.16	137.67	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	9003	SD2	CAY-NAX-CAS	9.98	143.97	121.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9002	SD2	9	0
3	B	9003	SD2	9	0

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	732/776 (94%)	-0.38	0	100 100	13, 39, 88, 93	0
1	B	734/776 (94%)	-0.39	1 (0%)	95 95	11, 38, 84, 96	0
All	All	1466/1552 (94%)	-0.39	1 (0%)	95 95	11, 38, 86, 96	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	LYS	2.2

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
3	SD2	A	9002	32/32	0.96	0.25	1.15	21,23,30,41	0
3	SD2	B	9003	32/32	0.96	0.23	0.58	16,23,32,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	B	9002	1/1	0.99	0.12	-1.60	17,17,17,17	0
2	ZN	A	9001	1/1	0.99	0.12	-1.69	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.