



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2019 – 07:54 PM EST

PDB ID : 6ED1
Title : Bacteroides dorei Beta-glucuronidase
Authors : Biernat, K.A.; Redinbo, M.R.
Deposited on : 2018-08-08
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

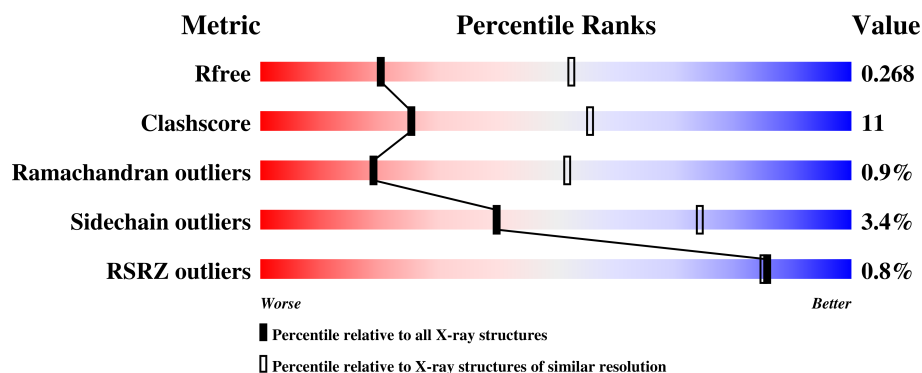
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

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	879	<div> <div>2%</div> <div>69% 27% ..</div> </div>
1	B	879	<div> <div>71% 26% ..</div> </div>
1	C	879	<div> <div>72% 24% ..</div> </div>
1	D	879	<div> <div>2%</div> <div>65% 31% ..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27956 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 Glycosyl hydrolase family 2, sugar binding domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	0	0
			6901	4411	1179	1281	30			
1	B	860	Total	C	N	O	S	0	0	0
			6914	4416	1181	1287	30			
1	C	860	Total	C	N	O	S	0	0	0
			6909	4413	1178	1289	29			
1	D	860	Total	C	N	O	S	0	0	0
			6857	4382	1167	1279	29			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP C3R9X4
A	2	HIS	-	expression tag	UNP C3R9X4
A	3	HIS	-	expression tag	UNP C3R9X4
A	4	HIS	-	expression tag	UNP C3R9X4
A	5	HIS	-	expression tag	UNP C3R9X4
A	6	HIS	-	expression tag	UNP C3R9X4
A	7	HIS	-	expression tag	UNP C3R9X4
A	8	SER	-	expression tag	UNP C3R9X4
A	9	SER	-	expression tag	UNP C3R9X4
A	10	GLY	-	expression tag	UNP C3R9X4
A	11	VAL	-	expression tag	UNP C3R9X4
A	12	ASP	-	expression tag	UNP C3R9X4
A	13	LEU	-	expression tag	UNP C3R9X4
A	14	GLY	-	expression tag	UNP C3R9X4
A	15	THR	-	expression tag	UNP C3R9X4
A	16	GLU	-	expression tag	UNP C3R9X4
A	17	ASN	-	expression tag	UNP C3R9X4
A	18	LEU	-	expression tag	UNP C3R9X4
A	19	TYR	-	expression tag	UNP C3R9X4
A	20	PHE	-	expression tag	UNP C3R9X4
A	21	GLN	-	expression tag	UNP C3R9X4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	-	expression tag	UNP C3R9X4
A	23	ASN	-	expression tag	UNP C3R9X4
B	1	MET	-	initiating methionine	UNP C3R9X4
B	2	HIS	-	expression tag	UNP C3R9X4
B	3	HIS	-	expression tag	UNP C3R9X4
B	4	HIS	-	expression tag	UNP C3R9X4
B	5	HIS	-	expression tag	UNP C3R9X4
B	6	HIS	-	expression tag	UNP C3R9X4
B	7	HIS	-	expression tag	UNP C3R9X4
B	8	SER	-	expression tag	UNP C3R9X4
B	9	SER	-	expression tag	UNP C3R9X4
B	10	GLY	-	expression tag	UNP C3R9X4
B	11	VAL	-	expression tag	UNP C3R9X4
B	12	ASP	-	expression tag	UNP C3R9X4
B	13	LEU	-	expression tag	UNP C3R9X4
B	14	GLY	-	expression tag	UNP C3R9X4
B	15	THR	-	expression tag	UNP C3R9X4
B	16	GLU	-	expression tag	UNP C3R9X4
B	17	ASN	-	expression tag	UNP C3R9X4
B	18	LEU	-	expression tag	UNP C3R9X4
B	19	TYR	-	expression tag	UNP C3R9X4
B	20	PHE	-	expression tag	UNP C3R9X4
B	21	GLN	-	expression tag	UNP C3R9X4
B	22	SER	-	expression tag	UNP C3R9X4
B	23	ASN	-	expression tag	UNP C3R9X4
C	1	MET	-	initiating methionine	UNP C3R9X4
C	2	HIS	-	expression tag	UNP C3R9X4
C	3	HIS	-	expression tag	UNP C3R9X4
C	4	HIS	-	expression tag	UNP C3R9X4
C	5	HIS	-	expression tag	UNP C3R9X4
C	6	HIS	-	expression tag	UNP C3R9X4
C	7	HIS	-	expression tag	UNP C3R9X4
C	8	SER	-	expression tag	UNP C3R9X4
C	9	SER	-	expression tag	UNP C3R9X4
C	10	GLY	-	expression tag	UNP C3R9X4
C	11	VAL	-	expression tag	UNP C3R9X4
C	12	ASP	-	expression tag	UNP C3R9X4
C	13	LEU	-	expression tag	UNP C3R9X4
C	14	GLY	-	expression tag	UNP C3R9X4
C	15	THR	-	expression tag	UNP C3R9X4
C	16	GLU	-	expression tag	UNP C3R9X4
C	17	ASN	-	expression tag	UNP C3R9X4

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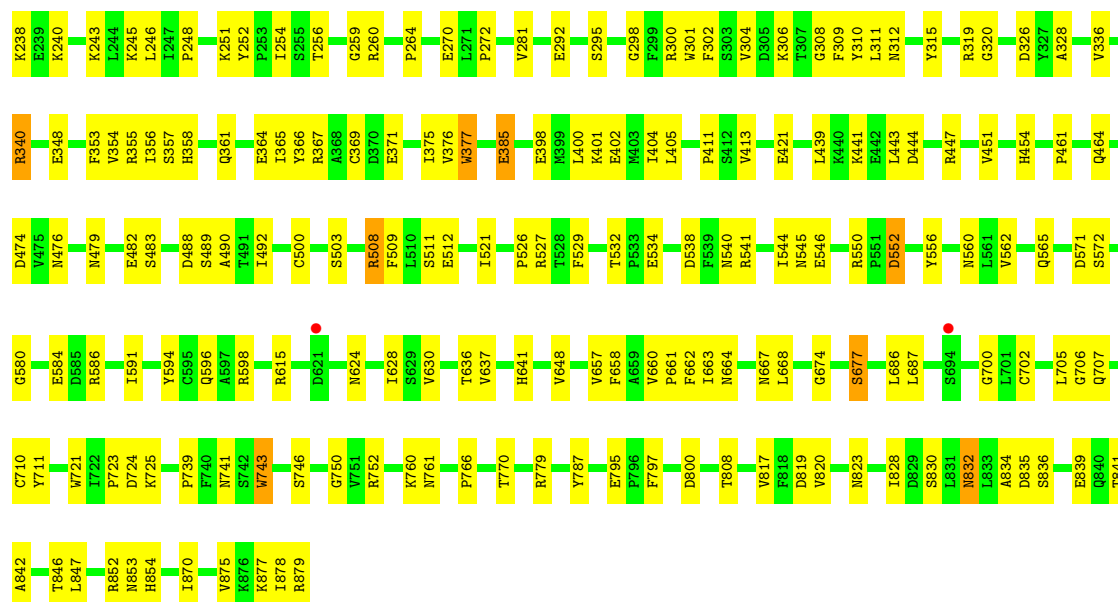
Chain	Residue	Modelled	Actual	Comment	Reference
C	18	LEU	-	expression tag	UNP C3R9X4
C	19	TYR	-	expression tag	UNP C3R9X4
C	20	PHE	-	expression tag	UNP C3R9X4
C	21	GLN	-	expression tag	UNP C3R9X4
C	22	SER	-	expression tag	UNP C3R9X4
C	23	ASN	-	expression tag	UNP C3R9X4
D	1	MET	-	initiating methionine	UNP C3R9X4
D	2	HIS	-	expression tag	UNP C3R9X4
D	3	HIS	-	expression tag	UNP C3R9X4
D	4	HIS	-	expression tag	UNP C3R9X4
D	5	HIS	-	expression tag	UNP C3R9X4
D	6	HIS	-	expression tag	UNP C3R9X4
D	7	HIS	-	expression tag	UNP C3R9X4
D	8	SER	-	expression tag	UNP C3R9X4
D	9	SER	-	expression tag	UNP C3R9X4
D	10	GLY	-	expression tag	UNP C3R9X4
D	11	VAL	-	expression tag	UNP C3R9X4
D	12	ASP	-	expression tag	UNP C3R9X4
D	13	LEU	-	expression tag	UNP C3R9X4
D	14	GLY	-	expression tag	UNP C3R9X4
D	15	THR	-	expression tag	UNP C3R9X4
D	16	GLU	-	expression tag	UNP C3R9X4
D	17	ASN	-	expression tag	UNP C3R9X4
D	18	LEU	-	expression tag	UNP C3R9X4
D	19	TYR	-	expression tag	UNP C3R9X4
D	20	PHE	-	expression tag	UNP C3R9X4
D	21	GLN	-	expression tag	UNP C3R9X4
D	22	SER	-	expression tag	UNP C3R9X4
D	23	ASN	-	expression tag	UNP C3R9X4

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

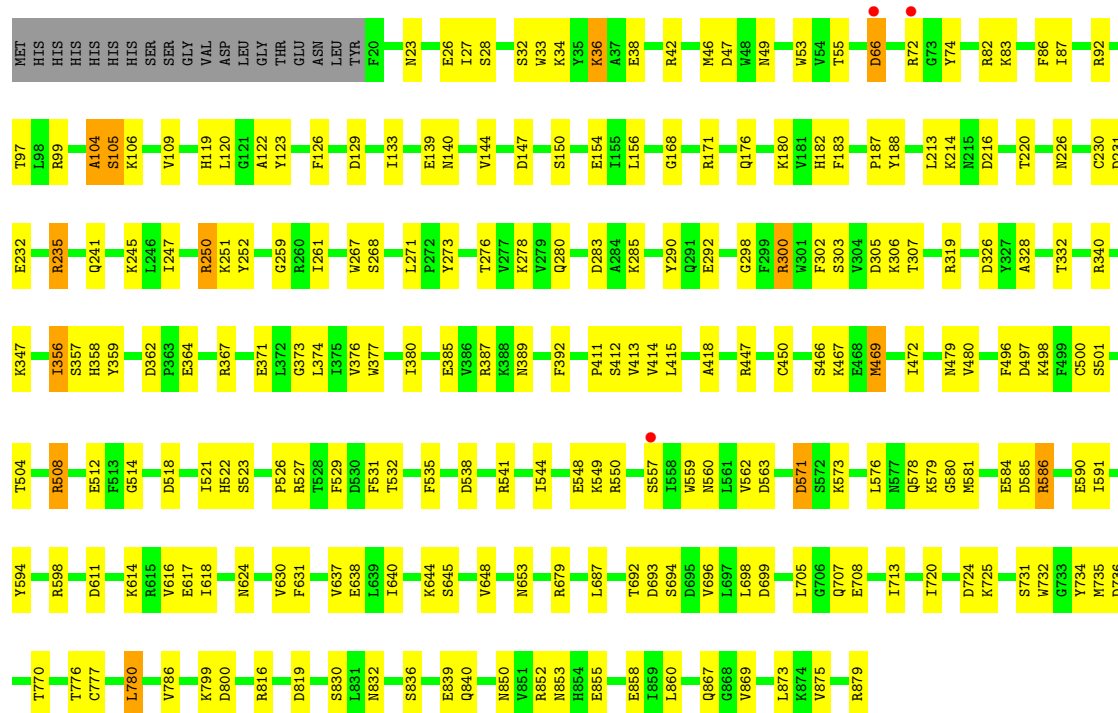
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	B	123	Total 123	O 123	0	0
3	C	80	Total 80	O 80	0	0
3	D	70	Total 70	O 70	0	0



- Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

Chain C: 72% 24% ..



- Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

Chain D: 2% 65% 31% ..



G838	K685	S572	I492	Q406	I294	V210	V103
T841	L686	G580	K498	K407	R300	A211	A104
L847	L687	M581	S501	Y408	W301	F212	S105
V848	L691	L582	Y502	S412	F302	L213	K106
V849	D693	R586	S503	L415	V304	K214	Y110
R852	S694	R587	T504	A418	D305	D216	L115
L860	D695	K588	A505	M419	K306	F217	L116
L861	V696	Y592	K506	N420	T307	T219	K117
S862	L705	Y593	P507	E421	G308	T220	T118
I870	G706	Y594	S511	D424	F309	H119	H119
V875	Y711	R598	E512	Y425	L311	L120	G121
K876	I720	D601	D518	H426	N312	G122	A122
K877	K725	P603	E519	Q428	F228	V227	I130
I878	R752	D611	R520	Q429	L229	L236	T131
R879	K760	V616	H522	L432	V237	V237	V136
	R761	E617	S523	E435	Q241	Q241	G137
	T762	I618	Y524	L436	L242	L242	E138
	F768	C619	T526	K441	K243	L244	E139
	T769	D620	T528	D444	L141	L141	N140
	T770	D621	F529	D445	L142	L142	L142
	T779	S622	F531	P445	R340	I247	K145
	R779	I623	T532	Y446	R341	P248	V146
	L780	N624	F533	R447	N352	P253	D147
	D781	V625	E534	L448	F353	I254	N148
	D784	R626	F535	C450	V854	S255	I155
	F791	S629	Q536	H454	R355	T256	L156
	F797	V630	L537	A455	I356	S257	P157
	R802	N633	N540	F456	I365	V258	F166
	K803	V637	R541	T457	D370	G259	F166
	T808	H641	I544	Y462	E371	I261	I169
	V817	R649	E546	T463	I375	E262	Y170
	F818	V657	K549	Q464	V376	P272	R171
	D819	P661	R550	S465	W377	Y273	R172
	V820	F662	P551	S466	S378	L274	K180
	S821	E666	Y553	K467	E379	V277	Y188
	V822	S673	I554	E468	I380	K278	V191
	D829	G674	F555	N469	K388	V279	P192
	N832	A675	G555	F470	H394	Q280	V193
	D835	L676	Y556	S471	N395	V281	R194
	S836	S677	S557	V475	E398	D282	I195
	Y837	K681	I558	M476	A284	D283	E199
			W559	G477	K285	K285	Y199
			N560	V478	N286	A287	A205
			D567	M479	L400	G287	S206
			G570	E482	E402	E288	P207
			D571	S483	M403	E292	Q208
					L405	V293	L209

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	242.66Å 101.36Å 168.60Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	29.54 – 2.90 29.54 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.54-2.90) 99.5 (29.54-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.178 , 0.268 0.178 , 0.268	Depositor DCC
R_{free} test set	1988 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27956	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/7071	0.62	0/9580
1	B	0.50	0/7084	0.64	0/9596
1	C	0.46	0/7079	0.61	0/9592
1	D	0.46	0/7027	0.62	0/9532
All	All	0.47	0/28261	0.62	0/38300

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	223	VAL	Peptide
1	D	303	SER	Peptide

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	6901	0	6764	152	2
1	B	6914	0	6771	142	0
1	C	6909	0	6760	156	0
1	D	6857	0	6660	183	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	98	0	0	6	0
3	B	123	0	0	6	0
3	C	80	0	0	7	0
3	D	70	0	0	8	0
All	All	27956	0	26955	621	2

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 11.

All (621) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:LEU:HD12	1:A:681:LYS:HG2	1.50	0.93
1:B:159:VAL:HG11	1:B:385:GLU:HG2	1.50	0.93
1:D:617:GLU:OE1	1:D:626:ARG:NH1	2.07	0.86
1:D:220:THR:HG22	1:D:247:ILE:HA	1.58	0.86
1:B:852:ARG:NH1	1:C:292:GLU:OE1	2.10	0.85
1:D:316:LEU:HD21	1:D:352:ASN:HD21	1.43	0.84
1:B:292:GLU:OE1	1:C:852:ARG:NH2	2.12	0.82
1:B:340:ARG:NH2	1:B:371:GLU:OE2	2.13	0.82
1:D:779:ARG:NH1	1:D:781:ASP:OD1	2.14	0.81
1:A:820:VAL:HG22	1:A:828:ILE:HB	1.61	0.81
1:D:649:ARG:NH1	3:D:1001:HOH:O	2.13	0.80
1:B:503:SER:O	1:B:508:ARG:NH1	2.15	0.80
1:D:694:SER:HB3	1:D:696:VAL:HG12	1.63	0.79
1:D:817:VAL:HG22	1:D:832:ASN:HB2	1.67	0.77
1:B:231:ASP:HB3	1:B:235:ARG:H	1.50	0.76
1:B:97:THR:HG23	1:B:176:GLN:HG3	1.66	0.76
1:D:306:LYS:NZ	1:D:504:THR:O	2.15	0.76
1:D:626:ARG:HG3	1:D:626:ARG:HH11	1.49	0.75
1:C:616:VAL:HG23	1:C:720:ILE:HD12	1.69	0.75
1:D:326:ASP:O	1:D:586:ARG:NH2	2.19	0.75
1:B:421:GLU:HG2	1:B:454:HIS:HB3	1.69	0.74
1:C:638:GLU:HB2	1:C:648:VAL:HG22	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:LYS:HD3	1:D:294:ILE:HG22	1.71	0.72
1:C:640:ILE:HA	1:C:645:SER:HA	1.72	0.70
1:B:156:LEU:HD12	1:B:157:PRO:HD2	1.73	0.70
1:B:820:VAL:HG22	1:B:828:ILE:HB	1.73	0.70
1:D:156:LEU:HD12	1:D:157:PRO:HD2	1.72	0.70
1:D:172:ARG:NH2	3:D:1007:HOH:O	2.25	0.70
1:A:449:SER:HB3	1:A:473:SER:HB3	1.74	0.69
1:A:802:ARG:HG2	1:A:808:THR:HG21	1.75	0.69
1:C:230:CYS:HB2	1:C:276:THR:HG22	1.73	0.69
1:D:102:GLY:HA3	1:D:171:ARG:HG3	1.73	0.68
1:D:215:ASN:HD21	1:D:217:PHE:HB2	1.58	0.68
1:D:797:PHE:O	1:D:802:ARG:NH1	2.26	0.68
1:B:706:GLY:HA2	1:B:739:PRO:HB3	1.76	0.68
1:C:47:ASP:O	3:C:1002:HOH:O	2.12	0.68
1:B:66:ASP:OD1	3:B:1002:HOH:O	2.12	0.68
1:D:621:ASP:OD1	1:D:622:SER:N	2.24	0.68
1:D:760:LYS:HB3	1:D:841:THR:HG22	1.73	0.68
1:A:816:ARG:NH1	1:A:867:GLN:O	2.27	0.67
1:C:303:SER:OG	3:C:1001:HOH:O	2.10	0.67
1:D:340:ARG:NH2	1:D:371:GLU:OE1	2.28	0.67
1:B:209:ILE:HG12	1:B:256:THR:HG22	1.76	0.67
1:A:105:SER:HB2	1:A:147:ASP:O	1.95	0.67
1:B:546:GLU:O	1:B:550:ARG:HG3	1.95	0.67
1:B:641:HIS:HE1	1:B:661:PRO:O	1.78	0.67
1:D:256:THR:HG22	1:D:257:SER:H	1.60	0.67
1:B:264:PRO:O	3:B:1003:HOH:O	2.13	0.66
1:D:521:ILE:HG22	1:D:532:THR:HG22	1.77	0.66
1:D:616:VAL:HG23	1:D:720:ILE:HD12	1.77	0.66
1:B:57:ASP:OD2	3:B:1001:HOH:O	2.12	0.66
1:C:42:ARG:HG3	1:C:42:ARG:HH11	1.60	0.66
1:A:355:ARG:HH12	1:A:512:GLU:HG3	1.61	0.66
1:C:319:ARG:NH1	1:C:548:GLU:OE2	2.28	0.66
1:A:614:LYS:HG3	1:A:720:ILE:HD11	1.78	0.65
1:B:356:ILE:HG23	1:B:361:GLN:HG3	1.77	0.65
1:C:326:ASP:HB3	1:C:332:THR:HG22	1.78	0.65
1:C:544:ILE:HG21	1:C:598:ARG:HE	1.61	0.65
1:A:663:ILE:HD12	1:A:664:ASN:O	1.96	0.65
1:D:518:ASP:HB3	1:D:521:ILE:HD12	1.77	0.65
1:A:581:MET:HE3	1:A:591:ILE:HG23	1.78	0.65
1:A:431:ALA:O	1:A:435:GLU:HG3	1.96	0.65
1:A:706:GLY:HA2	1:A:739:PRO:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LYS:HZ3	1:B:260:ARG:HG3	1.61	0.64
1:B:123:TYR:O	1:B:171:ARG:NH2	2.30	0.64
1:B:527:ARG:NH1	3:B:1006:HOH:O	2.30	0.64
1:D:570:GLY:O	3:D:1002:HOH:O	2.15	0.64
1:D:377:TRP:CE3	1:D:415:LEU:HD13	2.32	0.64
1:A:129:ASP:OD1	1:A:131:THR:HG22	1.98	0.64
1:B:761:ASN:HB3	1:B:842:ALA:HB3	1.79	0.63
1:A:123:TYR:O	1:A:171:ARG:NH2	2.31	0.63
1:C:598:ARG:HH12	1:C:653:ASN:HA	1.62	0.63
1:C:630:VAL:HG11	1:C:637:VAL:HG21	1.82	0.62
1:D:227:VAL:HG22	1:D:279:VAL:HG22	1.81	0.62
1:D:526:PRO:HG3	1:D:534:GLU:HB3	1.82	0.62
1:C:120:LEU:HB3	1:C:156:LEU:HD13	1.79	0.62
1:A:298:GLY:N	1:A:411:PRO:HG3	2.15	0.62
1:A:619:CYS:HB3	1:A:686:LEU:HD22	1.82	0.62
1:B:641:HIS:NE2	1:B:667:ASN:OD1	2.33	0.62
1:C:105:SER:H	1:C:122:ALA:HA	1.65	0.62
1:D:483:SER:HB2	1:D:492:ILE:HD11	1.82	0.62
1:A:340:ARG:NH2	1:A:371:GLU:OE2	2.32	0.62
1:A:603:PRO:HB2	1:A:676:LEU:HD11	1.81	0.62
1:D:155:ILE:O	1:D:395:ASN:ND2	2.33	0.62
1:D:194:ARG:H	1:D:194:ARG:HD2	1.64	0.62
1:A:826:LYS:NZ	3:A:1001:HOH:O	2.15	0.61
1:C:154:GLU:HG3	1:C:389:ASN:HD21	1.65	0.61
1:D:205:ALA:HB3	1:D:261:ILE:HB	1.82	0.61
1:D:498:LYS:O	1:D:501:SER:HB2	2.01	0.61
1:D:541:ARG:HB2	1:D:594:TYR:OH	2.01	0.61
1:A:408:TYR:HE1	1:A:444:ASP:HB2	1.63	0.61
1:A:829:ASP:O	1:A:830:SER:HB3	2.00	0.61
1:C:579:LYS:NZ	3:C:1007:HOH:O	2.34	0.61
1:C:581:MET:HE1	1:C:591:ILE:HG13	1.82	0.61
1:C:245:LYS:HE3	1:C:247:ILE:HD11	1.81	0.61
1:C:705:LEU:HD11	1:C:873:LEU:HB2	1.82	0.61
1:A:43:PHE:O	1:A:82:ARG:NH2	2.34	0.61
1:D:191:VAL:O	1:D:194:ARG:NH1	2.34	0.61
1:B:545:ASN:OD1	1:B:598:ARG:NH1	2.32	0.61
1:D:519:GLU:OE1	3:D:1003:HOH:O	2.16	0.61
1:D:603:PRO:HB2	1:D:676:LEU:HD11	1.84	0.60
1:D:540:ASN:O	1:D:544:ILE:HG12	2.02	0.60
1:D:309:PHE:HB2	1:D:554:ILE:HB	1.82	0.60
1:D:502:TYR:O	1:D:504:THR:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:VAL:HG22	1:D:507:PRO:HG3	1.82	0.60
1:A:569:ARG:NH2	3:A:1009:HOH:O	2.35	0.60
1:A:590:GLU:OE2	1:A:606:HIS:NE2	2.25	0.60
1:B:22:SER:HB3	1:C:850:ASN:O	2.00	0.60
1:B:707:GLN:HE21	1:B:770:THR:HG21	1.66	0.60
1:B:479:ASN:OD1	1:B:511:SER:HB2	2.02	0.59
1:B:401:LYS:HG2	1:B:443:LEU:HD11	1.83	0.59
1:D:427:LYS:N	1:D:427:LYS:HD3	2.17	0.59
1:B:172:ARG:NH2	3:B:1011:HOH:O	2.35	0.59
1:C:280:GLN:HG2	1:C:292:GLU:HG3	1.84	0.59
1:D:546:GLU:O	1:D:550:ARG:HD2	2.01	0.59
1:B:376:VAL:HB	1:B:413:VAL:HA	1.83	0.59
1:B:741:ASN:ND2	1:B:750:GLY:HA2	2.18	0.59
1:C:86:PHE:CE1	1:C:139:GLU:HB2	2.38	0.59
1:D:85:LEU:HD22	1:D:142:LEU:HD22	1.85	0.59
1:B:306:LYS:O	1:B:552:ASP:HA	2.03	0.59
1:B:560:ASN:O	1:B:580:GLY:HA2	2.03	0.59
1:B:367:ARG:NH2	1:C:698:LEU:O	2.34	0.59
1:D:415:LEU:HD22	1:D:450:CYS:HB3	1.84	0.59
1:C:500:CYS:HB3	1:C:508:ARG:HH21	1.66	0.59
1:D:191:VAL:HG23	1:D:405:LEU:O	2.03	0.58
1:A:96:ILE:H	1:A:131:THR:HB	1.68	0.58
1:C:617:GLU:OE2	1:C:624:ASN:ND2	2.34	0.58
1:A:639:LEU:HD23	1:A:646:LEU:HD12	1.86	0.58
1:A:222:HIS:NE2	1:A:245:LYS:HD2	2.18	0.58
1:C:725:LYS:HE2	1:C:732:TRP:O	2.04	0.58
1:B:461:PRO:HA	1:B:464:GLN:HG3	1.85	0.58
1:A:759:ILE:HD12	1:A:794:THR:HG21	1.86	0.58
1:C:66:ASP:HB3	1:C:74:TYR:HB2	1.86	0.58
1:D:219:ASP:O	1:D:248:PRO:HG3	2.04	0.58
1:C:512:GLU:HB2	1:C:559:TRP:HB2	1.85	0.57
1:C:387:ARG:HB2	1:C:392:PHE:CD1	2.39	0.57
1:D:526:PRO:HB2	1:D:535:PHE:HB2	1.86	0.57
1:B:710:CYS:O	1:B:723:PRO:HG3	2.05	0.57
1:A:638:GLU:HB2	1:A:648:VAL:HG22	1.86	0.57
1:C:226:ASN:OD1	1:C:241:GLN:NE2	2.33	0.57
1:B:482:GLU:O	1:B:483:SER:HB3	2.04	0.57
1:D:236:ILE:HD12	1:D:236:ILE:H	1.69	0.57
1:B:852:ARG:NH2	1:C:23:ASN:OD1	2.38	0.57
1:D:67:VAL:HG13	1:D:567:ASP:HB2	1.86	0.57
1:A:518:ASP:HB3	1:A:521:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:VAL:HG11	1:B:637:VAL:HG21	1.86	0.56
1:D:80:TRP:CE2	1:D:145:LYS:HG3	2.40	0.56
1:A:588:LYS:HD3	1:A:592:TYR:CE2	2.40	0.56
1:B:795:GLU:HB3	1:B:839:GLU:HA	1.86	0.56
1:A:634:GLN:HB3	3:A:1039:HOH:O	2.04	0.56
1:A:498:LYS:O	1:A:501:SER:HB2	2.06	0.56
1:A:74:TYR:CE1	1:A:76:ARG:HD3	2.41	0.56
1:A:798:SER:OG	1:A:801:GLU:HG3	2.05	0.56
1:B:105:SER:H	1:B:122:ALA:HB2	1.71	0.56
1:B:115:LEU:HD11	1:B:118:THR:HG22	1.88	0.56
1:B:817:VAL:HG22	1:B:832:ASN:HB2	1.85	0.56
1:C:526:PRO:O	1:C:527:ARG:HD3	2.06	0.56
1:C:531:PHE:CZ	1:C:571:ASP:HB3	2.41	0.56
1:C:694:SER:HB3	1:C:696:VAL:HG12	1.88	0.56
1:D:603:PRO:HA	1:D:633:ASN:HD22	1.70	0.56
1:A:466:SER:OG	1:A:467:LYS:N	2.38	0.56
1:D:791:PHE:CE2	1:D:847:LEU:HD12	2.41	0.56
1:A:34:LYS:HD2	1:A:53:TRP:HB2	1.87	0.56
1:A:791:PHE:O	1:A:844:VAL:HA	2.05	0.56
1:A:36:LYS:HE3	1:A:53:TRP:CD1	2.41	0.55
1:A:538:ASP:OD2	1:A:541:ARG:NH1	2.39	0.55
1:A:787:TYR:CZ	1:A:877:LYS:HG3	2.41	0.55
1:C:34:LYS:HD3	1:C:55:THR:HG22	1.87	0.55
1:D:147:ASP:OD1	1:D:148:ASN:N	2.39	0.55
1:A:440:LYS:HD2	1:A:449:SER:OG	2.06	0.55
1:C:119:HIS:CD2	1:C:126:PHE:HB3	2.41	0.55
1:D:305:ASP:CG	1:D:307:THR:HG22	2.26	0.55
1:A:726:PRO:HG3	1:A:734:TYR:CZ	2.42	0.55
1:A:649:ARG:HG3	1:A:658:PHE:CE1	2.41	0.55
1:B:208:GLN:NE2	1:B:256:THR:O	2.39	0.55
1:A:672:ARG:HG2	1:A:677:SER:HB3	1.88	0.55
1:B:377:TRP:HZ3	1:B:509:PHE:CD1	2.25	0.55
1:A:811:SER:O	1:A:814:GLY:N	2.24	0.55
1:D:705:LEU:HD12	1:D:870:ILE:HG12	1.88	0.55
1:A:616:VAL:HG22	1:A:685:LYS:HB3	1.89	0.55
1:D:316:LEU:HD21	1:D:352:ASN:ND2	2.19	0.54
1:C:305:ASP:OD1	1:C:307:THR:HG22	2.08	0.54
1:C:340:ARG:NH2	1:C:371:GLU:OE2	2.40	0.54
1:D:618:ILE:HD13	1:D:725:LYS:HE3	1.90	0.54
1:D:832:ASN:O	1:D:836:SER:HB2	2.07	0.54
1:A:99:ARG:HD3	1:A:174:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:LEU:HB3	1:A:772:LEU:HD12	1.89	0.54
1:C:133:ILE:H	1:C:133:ILE:HD12	1.72	0.54
1:A:436:LEU:O	1:A:440:LYS:HG3	2.07	0.53
1:B:77:GLY:H	1:B:148:ASN:HB3	1.73	0.53
1:C:736:ASP:OD2	1:C:776:THR:OG1	2.26	0.53
1:A:192:PRO:HG2	1:A:293:VAL:HG11	1.89	0.53
1:A:33:TRP:CE3	1:A:81:TYR:HB3	2.42	0.53
1:D:311:LEU:HD13	1:D:375:ILE:HD11	1.90	0.53
1:D:466:SER:OG	1:D:467:LYS:N	2.41	0.53
1:D:544:ILE:HD12	1:D:556:TYR:CE2	2.43	0.53
1:A:103:VAL:HG22	1:A:169:ILE:HG23	1.91	0.53
1:A:736:ASP:OD1	1:A:737:GLY:N	2.42	0.53
1:D:305:ASP:OD1	1:D:307:THR:HG22	2.09	0.53
1:B:80:TRP:CE2	1:B:145:LYS:HG3	2.44	0.53
1:C:415:LEU:HB3	1:C:450:CYS:SG	2.49	0.53
1:C:526:PRO:HB2	1:C:535:PHE:HB2	1.90	0.53
1:B:677:SER:HB3	1:C:679:ARG:HH22	1.74	0.53
1:D:469:MET:N	1:D:469:MET:SD	2.81	0.53
1:A:120:LEU:HB3	1:A:156:LEU:HD13	1.90	0.53
1:A:541:ARG:NH1	3:A:1002:HOH:O	2.42	0.53
1:A:725:LYS:NZ	1:A:728:THR:HG22	2.23	0.53
1:B:62:TRP:HZ2	1:B:148:ASN:HB2	1.74	0.53
1:D:380:ILE:HD11	1:D:400:LEU:HD12	1.91	0.53
1:D:394:HIS:O	1:D:398:GLU:HG2	2.09	0.53
1:B:308:GLY:HA3	1:B:315:TYR:HE1	1.74	0.52
1:D:784:ASP:O	1:D:877:LYS:NZ	2.41	0.52
1:D:63:ASN:HA	1:D:66:ASP:HB2	1.91	0.52
1:A:228:PHE:HB2	1:A:278:LYS:HB3	1.92	0.52
1:C:523:SER:HB2	1:C:532:THR:HG21	1.91	0.52
1:C:541:ARG:HG2	1:C:594:TYR:OH	2.09	0.52
1:D:518:ASP:OD1	1:D:572:SER:OG	2.27	0.52
1:B:677:SER:HB3	1:C:679:ARG:HH12	1.74	0.52
1:B:238:LYS:NZ	1:B:260:ARG:HG3	2.24	0.52
1:C:376:VAL:HB	1:C:413:VAL:HA	1.91	0.52
1:D:415:LEU:HB3	1:D:450:CYS:SG	2.49	0.52
1:A:29:ILE:HD11	1:A:173:VAL:HG12	1.92	0.52
1:A:424:ASP:OD1	1:A:460:LYS:HE3	2.10	0.52
1:C:562:VAL:HG11	1:C:586:ARG:NH1	2.24	0.52
1:D:256:THR:HG22	1:D:257:SER:N	2.24	0.52
1:D:307:THR:HG23	1:D:310:TYR:OH	2.10	0.52
1:D:90:GLU:HG3	1:D:90:GLU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ARG:HG3	1:C:42:ARG:NH1	2.25	0.52
1:C:97:THR:HG22	1:C:129:ASP:HA	1.91	0.52
1:A:815:GLN:OE1	1:A:865:LYS:NZ	2.41	0.52
1:D:208:GLN:HA	1:D:257:SER:HA	1.91	0.52
1:D:45:SER:HB2	1:D:48:TRP:HB2	1.91	0.52
1:A:298:GLY:H	1:A:411:PRO:HG3	1.75	0.52
1:A:822:VAL:HG12	1:A:827:LEU:HD23	1.92	0.52
1:A:222:HIS:CE1	1:A:245:LYS:HD2	2.45	0.51
1:C:497:ASP:OD1	1:C:550:ARG:NH1	2.42	0.51
1:D:529:PHE:HB3	1:D:752:ARG:HD2	1.93	0.51
1:B:224:HIS:ND1	1:B:243:LYS:HG2	2.25	0.51
1:B:104:ALA:HB3	1:B:167:GLY:HA2	1.92	0.51
1:D:274:LEU:HD21	1:D:370:ASP:HB2	1.93	0.51
1:C:527:ARG:NH2	3:C:1008:HOH:O	2.42	0.51
1:D:707:GLN:HB2	1:D:770:THR:HG21	1.92	0.51
1:A:76:ARG:NE	1:A:148:ASN:O	2.40	0.51
1:A:413:VAL:HG11	1:A:416:TRP:CH2	2.46	0.51
1:C:585:ASP:O	1:C:586:ARG:HB2	2.10	0.51
1:D:105:SER:HB2	1:D:147:ASP:O	2.11	0.51
1:D:304:VAL:HG22	1:D:507:PRO:CG	2.41	0.51
1:A:408:TYR:CE1	1:A:444:ASP:HB2	2.45	0.51
1:A:481:TYR:OH	1:A:512:GLU:OE2	2.29	0.51
1:D:421:GLU:HG3	1:D:479:ASN:ND2	2.26	0.51
1:B:319:ARG:HG2	1:B:556:TYR:CE1	2.46	0.50
1:C:479:ASN:CG	1:C:512:GLU:HG2	2.32	0.50
1:B:328:ALA:HB2	1:B:584:GLU:HG3	1.93	0.50
1:D:215:ASN:ND2	1:D:217:PHE:HB2	2.25	0.50
1:A:510:LEU:HB3	1:A:556:TYR:CB	2.41	0.50
1:B:320:GLY:HA3	1:B:353:PHE:O	2.11	0.50
1:B:521:ILE:HG22	1:B:532:THR:HG22	1.92	0.50
1:D:457:THR:HA	1:D:462:TYR:CD2	2.46	0.50
1:B:636:THR:HG23	1:B:648:VAL:HG13	1.93	0.50
1:C:105:SER:O	3:C:1003:HOH:O	2.20	0.50
1:C:560:ASN:O	1:C:580:GLY:HA2	2.11	0.50
1:C:692:THR:OG1	1:C:693:ASP:OD1	2.28	0.50
1:D:105:SER:H	1:D:122:ALA:HB2	1.77	0.50
1:D:432:LEU:HA	1:D:435:GLU:OE1	2.11	0.50
1:A:27:ILE:HG22	1:A:177:TRP:HZ3	1.77	0.50
1:A:791:PHE:HB3	1:A:793:PHE:CE2	2.47	0.50
1:A:827:LEU:HG	1:A:847:LEU:HD22	1.94	0.50
1:C:816:ARG:HD3	1:C:867:GLN:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:624:ASN:O	1:D:662:PHE:HB2	2.12	0.50
1:B:398:GLU:O	1:B:402:GLU:HG3	2.11	0.49
1:B:400:LEU:HD23	1:B:439:LEU:HD23	1.93	0.49
1:C:214:LYS:HE2	1:C:251:LYS:HG2	1.93	0.49
1:B:87:ILE:HG22	1:B:136:VAL:HG13	1.94	0.49
1:D:229:LEU:O	1:D:237:VAL:HG22	2.12	0.49
1:A:532:THR:HB	1:A:534:GLU:OE1	2.11	0.49
1:D:819:ASP:HB2	1:D:862:SER:OG	2.12	0.49
1:C:816:ARG:HD2	1:C:869:VAL:HG22	1.95	0.49
1:D:82:ARG:NH2	1:D:141:LEU:HD21	2.27	0.49
1:A:380:ILE:HG13	1:A:418:ALA:HA	1.94	0.49
1:A:110:TYR:CE2	1:A:115:LEU:HB2	2.47	0.49
1:B:164:SER:HB2	1:B:166:PHE:CE1	2.47	0.49
1:C:267:TRP:CH2	1:C:412:SER:HA	2.48	0.49
1:D:549:LYS:O	1:D:551:PRO:HD3	2.12	0.49
1:B:211:ALA:HB3	1:B:254:ILE:HD11	1.95	0.49
1:D:180:LYS:HB2	1:D:217:PHE:CE2	2.47	0.49
1:C:180:LYS:HB3	1:C:216:ASP:HB2	1.95	0.49
1:A:794:THR:HG23	1:A:840:GLN:HA	1.95	0.49
1:C:306:LYS:NZ	1:C:504:THR:O	2.42	0.49
1:C:581:MET:HE3	1:C:591:ILE:HG23	1.95	0.49
1:B:103:VAL:HG22	1:B:126:PHE:HE2	1.78	0.48
1:B:444:ASP:OD2	1:B:447:ARG:HD2	2.13	0.48
1:B:664:ASN:HB2	1:B:686:LEU:HD12	1.95	0.48
1:D:278:LYS:HD3	1:D:294:ILE:CG2	2.42	0.48
1:A:261:ILE:O	1:A:262:GLU:HB2	2.14	0.48
1:A:614:LYS:HG3	1:A:720:ILE:CD1	2.42	0.48
1:B:663:ILE:HD12	1:B:664:ASN:O	2.12	0.48
1:C:518:ASP:HB3	1:C:521:ILE:HD12	1.94	0.48
1:D:629:SER:HB3	1:D:657:VAL:HG22	1.94	0.48
1:B:246:LEU:HA	1:B:252:TYR:CE2	2.47	0.48
1:C:123:TYR:O	1:C:171:ARG:NH2	2.45	0.48
1:C:171:ARG:HD2	1:C:362:ASP:OD1	2.14	0.48
1:C:298:GLY:N	1:C:411:PRO:HG3	2.27	0.48
1:C:644:LYS:HD3	1:C:644:LYS:HA	1.49	0.48
1:B:308:GLY:HA3	1:B:315:TYR:CE1	2.48	0.48
1:D:832:ASN:ND2	3:D:1019:HOH:O	2.47	0.48
1:A:229:LEU:O	1:A:237:VAL:HG22	2.13	0.48
1:C:498:LYS:O	1:C:501:SER:HB3	2.12	0.48
1:C:713:ILE:HG13	1:C:720:ILE:HG12	1.94	0.48
1:D:117:LYS:HG3	1:D:118:THR:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ASP:HB3	1:D:286:ASN:HB3	1.93	0.48
1:D:821:SER:HB2	1:D:860:LEU:HD12	1.95	0.48
1:A:423:TRP:O	1:A:460:LYS:HB2	2.13	0.48
1:D:279:VAL:O	1:D:292:GLU:HA	2.13	0.48
1:D:630:VAL:HG11	1:D:637:VAL:HG11	1.94	0.48
1:A:560:ASN:O	1:A:580:GLY:HA2	2.14	0.48
1:A:725:LYS:HZ1	1:A:728:THR:HG22	1.79	0.48
1:A:817:VAL:HA	1:A:831:LEU:O	2.14	0.48
1:D:388:LYS:HE3	1:D:428:GLN:OE1	2.14	0.48
1:A:457:THR:HG21	1:A:498:LYS:HD3	1.96	0.48
1:B:103:VAL:HG12	1:B:169:ILE:HG23	1.96	0.48
1:D:110:TYR:CE2	1:D:115:LEU:HB2	2.49	0.48
1:D:106:LYS:HG3	1:D:120:LEU:HD23	1.95	0.48
1:D:195:ILE:CD1	1:D:277:VAL:HG11	2.43	0.48
1:D:822:VAL:HG11	1:D:849:VAL:HG21	1.96	0.48
1:A:355:ARG:NH1	1:A:512:GLU:HG3	2.27	0.48
1:C:87:ILE:HD12	1:C:140:ASN:ND2	2.29	0.48
1:B:25:SER:HB2	1:C:850:ASN:HD21	1.79	0.47
1:D:522:HIS:NE2	1:D:611:ASP:OD2	2.38	0.47
1:D:666:GLU:OE2	1:D:681:LYS:HD3	2.14	0.47
1:A:468:GLU:HG2	1:D:446:TYR:OH	2.14	0.47
1:B:105:SER:H	1:B:122:ALA:CB	2.27	0.47
1:C:522:HIS:NE2	1:C:611:ASP:OD2	2.35	0.47
1:D:355:ARG:NE	1:D:379:GLU:OE2	2.43	0.47
1:D:524:TYR:CE1	1:D:626:ARG:NH1	2.83	0.47
1:B:624:ASN:O	1:B:662:PHE:HB2	2.14	0.47
1:D:193:VAL:HG23	1:D:210:VAL:O	2.14	0.47
1:C:356:ILE:HG12	1:C:376:VAL:HG13	1.96	0.47
1:A:797:PHE:HB3	1:A:801:GLU:HB2	1.96	0.47
1:B:172:ARG:NH2	1:B:336:VAL:HG21	2.30	0.47
1:B:355:ARG:NH1	1:B:512:GLU:HG3	2.30	0.47
1:B:60:HIS:ND1	1:B:81:TYR:OH	2.40	0.47
1:D:685:LYS:HE3	1:D:687:LEU:HD21	1.95	0.47
1:A:355:ARG:NH1	1:A:511:SER:HB2	2.30	0.47
1:C:231:ASP:HB3	1:C:235:ARG:H	1.80	0.47
1:C:347:LYS:HB2	1:C:374:LEU:HD11	1.97	0.47
1:B:846:THR:C	1:B:847:LEU:HD12	2.35	0.47
1:B:222:HIS:NE2	1:B:245:LYS:HG3	2.29	0.47
1:B:62:TRP:CZ2	1:B:148:ASN:HB2	2.50	0.47
1:C:302:PHE:HZ	1:C:447:ARG:HA	1.80	0.47
1:D:380:ILE:HG13	1:D:418:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:641:HIS:HE1	1:D:661:PRO:O	1.97	0.47
1:A:94:LYS:HB3	1:A:178:THR:O	2.15	0.47
1:B:364:GLU:OE1	1:B:367:ARG:NH1	2.44	0.47
1:B:500:CYS:HB3	1:B:508:ARG:NH2	2.29	0.47
1:B:705:LEU:HD12	1:B:870:ILE:HG12	1.95	0.47
1:B:832:ASN:OD1	1:B:835:ASP:HB2	2.14	0.47
1:B:853:ASN:OD1	1:B:854:HIS:N	2.48	0.47
1:A:797:PHE:CG	1:A:808:THR:HG23	2.50	0.47
1:D:466:SER:OG	1:D:468:GLU:N	2.41	0.47
1:B:166:PHE:HD1	1:B:166:PHE:H	1.62	0.47
1:B:795:GLU:HG2	1:B:834:ALA:HB2	1.97	0.47
1:C:46:MET:HG2	3:C:1029:HOH:O	2.15	0.47
1:D:587:ARG:NH2	3:D:1003:HOH:O	2.42	0.47
1:B:355:ARG:HH12	1:B:512:GLU:HG3	1.80	0.46
1:C:614:LYS:HE3	1:C:614:LYS:HB3	1.81	0.46
1:C:598:ARG:NH1	1:C:653:ASN:CA	2.78	0.46
1:D:376:VAL:HG23	1:D:412:SER:HB2	1.97	0.46
1:A:466:SER:OG	1:A:468:GLU:HG3	2.15	0.46
1:A:510:LEU:HB3	1:A:556:TYR:HB2	1.96	0.46
1:C:598:ARG:HG2	1:C:598:ARG:HH11	1.81	0.46
1:D:780:LEU:HD22	1:D:875:VAL:HG21	1.97	0.46
1:B:304:VAL:HG12	1:B:309:PHE:HD1	1.79	0.46
1:D:588:LYS:HD3	1:D:592:TYR:CE2	2.50	0.46
1:A:795:GLU:HG2	1:A:834:ALA:HB2	1.97	0.46
1:C:357:SER:HB2	1:C:358:HIS:ND1	2.31	0.46
1:A:46:MET:HA	1:A:141:LEU:HD22	1.98	0.46
1:C:104:ALA:HB3	1:C:168:GLY:H	1.80	0.46
1:C:598:ARG:HH12	1:C:653:ASN:CA	2.26	0.46
1:C:66:ASP:HB3	1:C:74:TYR:CB	2.44	0.46
1:C:26:GLU:OE2	1:C:99:ARG:NH1	2.49	0.46
1:D:797:PHE:CG	1:D:808:THR:HG22	2.50	0.46
1:C:300:ARG:HH22	1:C:302:PHE:HE1	1.63	0.46
1:A:120:LEU:HB3	1:A:156:LEU:CD1	2.46	0.46
1:A:280:GLN:HG2	1:A:292:GLU:HG3	1.98	0.46
1:C:86:PHE:CZ	1:C:139:GLU:HB2	2.50	0.46
1:D:46:MET:HA	1:D:141:LEU:HD22	1.98	0.46
1:D:617:GLU:HG2	1:D:711:TYR:CE1	2.51	0.46
1:A:415:LEU:HB3	1:A:450:CYS:SG	2.56	0.46
1:B:743:TRP:HZ3	1:B:752:ARG:O	1.99	0.46
1:C:708:GLU:OE2	1:C:734:TYR:OH	2.20	0.46
1:A:231:ASP:OD2	1:A:235:ARG:NH1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:TRP:HZ2	1:A:486:GLN:NE2	2.14	0.46
1:C:594:TYR:CZ	1:C:598:ARG:HD2	2.51	0.46
1:A:367:ARG:NH1	3:A:1019:HOH:O	2.48	0.46
1:C:123:TYR:CG	1:C:359:TYR:HB2	2.51	0.46
1:C:694:SER:C	1:C:696:VAL:H	2.19	0.46
1:D:402:GLU:HG2	1:D:406:GLN:NE2	2.31	0.46
1:A:302:PHE:CE2	1:A:414:VAL:HG13	2.50	0.45
1:A:190:ALA:HB2	1:A:405:LEU:HB3	1.98	0.45
1:A:797:PHE:CD2	1:A:808:THR:HG23	2.51	0.45
1:D:188:TYR:HD1	1:D:402:GLU:HG3	1.80	0.45
1:D:531:PHE:CZ	1:D:571:ASP:HB3	2.51	0.45
1:A:401:LYS:HG2	1:A:443:LEU:HD21	1.99	0.45
1:A:444:ASP:OD2	1:A:447:ARG:HD2	2.16	0.45
1:B:200:VAL:HG13	1:B:205:ALA:HB2	1.98	0.45
1:B:240:LYS:HD3	1:B:256:THR:OG1	2.17	0.45
1:B:238:LYS:NZ	1:B:259:GLY:O	2.48	0.45
1:C:389:ASN:HB2	1:C:392:PHE:HB2	1.96	0.45
1:C:36:LYS:HG2	1:C:38:GLU:HB3	1.98	0.45
1:D:444:ASP:OD2	1:D:447:ARG:NH1	2.42	0.45
1:D:432:LEU:O	1:D:436:LEU:HG	2.16	0.45
1:C:278:LYS:HD3	1:C:292:GLU:OE2	2.16	0.45
1:C:576:LEU:HD23	1:C:578:GLN:HG2	1.99	0.45
1:B:847:LEU:HG	1:C:27:ILE:HD12	1.99	0.45
1:C:853:ASN:HB3	1:C:855:GLU:HG3	1.97	0.45
1:D:355:ARG:NH2	1:D:420:ASN:OD1	2.50	0.45
1:A:697:LEU:HB3	1:A:877:LYS:HB2	1.98	0.45
1:B:272:PRO:HG2	3:B:1042:HOH:O	2.17	0.45
1:B:326:ASP:OD2	1:B:565:GLN:NE2	2.46	0.45
1:D:206:SER:HA	1:D:259:GLY:HA2	1.98	0.45
1:D:475:VAL:HG11	1:D:554:ILE:HD11	1.97	0.45
1:A:668:LEU:CD1	1:A:681:LYS:HE2	2.47	0.45
1:A:707:GLN:HE21	1:A:770:THR:HG21	1.81	0.45
1:B:878:ILE:O	1:B:879:ARG:HB3	2.17	0.45
1:C:544:ILE:CG2	1:C:598:ARG:HE	2.28	0.45
1:A:70:GLU:CD	1:A:760:LYS:HG2	2.37	0.45
1:B:441:LYS:NZ	1:B:474:ASP:OD2	2.50	0.45
1:B:541:ARG:HG3	1:B:594:TYR:OH	2.16	0.45
1:C:182:HIS:CE1	1:C:214:LYS:HD2	2.52	0.45
1:D:558:ILE:HG21	1:D:581:MET:SD	2.57	0.45
1:A:545:ASN:OD1	1:A:598:ARG:NH1	2.23	0.45
1:A:635:LYS:NZ	3:A:1022:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:LEU:HD22	1:B:375:ILE:HD11	1.97	0.45
1:B:171:ARG:HH12	1:B:361:GLN:HA	1.83	0.44
1:C:414:VAL:HG12	1:C:415:LEU:HD12	1.98	0.44
1:C:328:ALA:HB2	1:C:584:GLU:HG3	1.99	0.44
1:C:594:TYR:HB2	1:C:631:PHE:CE2	2.53	0.44
1:D:582:LEU:HD23	1:D:588:LYS:HA	1.99	0.44
1:A:687:LEU:HD21	1:A:696:VAL:HG21	1.99	0.44
1:C:106:LYS:HB3	1:C:147:ASP:HB3	1.98	0.44
1:C:154:GLU:HG3	1:C:154:GLU:O	2.17	0.44
1:A:242:LEU:HD11	1:A:256:THR:OG1	2.17	0.44
1:A:727:TYR:CE1	1:A:779:ARG:HB2	2.52	0.44
1:A:820:VAL:HG22	1:A:828:ILE:CB	2.40	0.44
1:C:469:MET:HA	1:C:472:ILE:CD1	2.48	0.44
1:B:301:TRP:CE2	1:B:312:ASN:HA	2.51	0.44
1:B:400:LEU:O	1:B:404:ILE:HG13	2.18	0.44
1:C:573:LYS:NZ	3:C:1009:HOH:O	2.43	0.44
1:D:103:VAL:HG22	1:D:169:ILE:HG23	1.99	0.44
1:A:545:ASN:O	1:A:549:LYS:HG2	2.17	0.44
1:C:268:SER:HB3	1:C:271:LEU:H	1.83	0.44
1:C:731:SER:OG	1:C:732:TRP:N	2.50	0.44
1:D:195:ILE:HD13	1:D:277:VAL:HG11	1.99	0.44
1:D:482:GLU:HB2	1:D:492:ILE:HG12	1.99	0.44
1:D:581:MET:HE3	1:D:581:MET:HB3	1.52	0.44
1:D:637:VAL:HA	1:D:673:SER:HB2	1.98	0.44
1:A:858:GLU:OE1	1:A:860:LEU:HD11	2.18	0.44
1:C:387:ARG:HB2	1:C:392:PHE:CG	2.53	0.44
1:A:444:ASP:OD2	1:A:447:ARG:HB2	2.17	0.44
1:C:278:LYS:HB2	1:C:278:LYS:HE2	1.63	0.44
1:B:213:LEU:HD21	1:B:281:VAL:HG21	2.00	0.44
1:C:562:VAL:HG12	1:C:563:ASP:O	2.18	0.44
1:D:838:GLY:O	1:D:841:THR:OG1	2.36	0.44
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.86	0.44
1:B:23:ASN:ND2	1:C:852:ARG:NH1	2.66	0.44
1:C:480:VAL:HG21	1:C:496:PHE:HE2	1.83	0.44
1:A:430:ILE:HG12	1:A:430:ILE:H	1.65	0.43
1:A:540:ASN:ND2	1:A:591:ILE:HD11	2.33	0.43
1:B:302:PHE:HA	1:B:310:TYR:O	2.19	0.43
1:B:540:ASN:O	1:B:544:ILE:HD12	2.18	0.43
1:D:380:ILE:HG23	1:D:403:MET:SD	2.58	0.43
1:D:441:LYS:HA	1:D:444:ASP:O	2.18	0.43
1:C:187:PRO:HG2	1:C:188:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:VAL:HG21	1:D:475:VAL:HG22	2.01	0.43
1:D:559:TRP:HA	1:D:560:ASN:HA	1.74	0.43
1:D:56:VAL:HG11	1:D:60:HIS:CD2	2.54	0.43
1:A:340:ARG:HE	1:A:367:ARG:HH12	1.67	0.43
1:A:604:MET:HE2	1:A:632:SER:HA	2.00	0.43
1:B:152:LEU:C	1:B:154:GLU:H	2.20	0.43
1:B:724:ASP:OD1	1:B:725:LYS:N	2.50	0.43
1:D:691:LEU:HD23	1:D:691:LEU:HA	1.78	0.43
1:A:482:GLU:O	1:A:483:SER:HB3	2.19	0.43
1:B:357:SER:HB2	1:B:358:HIS:HA	2.01	0.43
1:B:365:ILE:HG22	1:B:366:TYR:CD2	2.54	0.43
1:B:797:PHE:CD1	1:B:808:THR:HG22	2.53	0.43
1:B:832:ASN:O	1:B:836:SER:HB2	2.18	0.43
1:A:99:ARG:HB3	1:A:174:PHE:HB2	2.00	0.43
1:A:559:TRP:HA	1:A:560:ASN:HA	1.78	0.43
1:D:455:ALA:HB2	1:D:478:VAL:HG22	2.00	0.43
1:D:61:THR:OG1	1:D:166:PHE:HB3	2.19	0.43
1:A:225:VAL:O	1:A:241:GLN:HA	2.18	0.43
1:A:664:ASN:HB2	1:A:686:LEU:HD12	1.99	0.43
1:B:377:TRP:CZ3	1:B:509:PHE:CD1	3.06	0.43
1:B:572:SER:HB2	1:B:766:PRO:HG3	2.00	0.43
1:C:36:LYS:HD2	1:C:53:TRP:CE2	2.53	0.43
1:C:590:GLU:HG2	1:C:611:ASP:OD1	2.18	0.43
1:C:707:GLN:HB2	1:C:770:THR:HG21	2.01	0.43
1:C:735:MET:HG3	1:C:777:CYS:SG	2.58	0.43
1:C:786:VAL:HB	1:C:879:ARG:HG3	1.99	0.43
1:D:308:GLY:C	1:D:554:ILE:HG22	2.39	0.43
1:D:48:TRP:CG	1:D:49:ASN:N	2.87	0.43
1:D:832:ASN:OD1	1:D:835:ASP:HB2	2.19	0.43
1:D:84:LYS:HD3	1:D:139:GLU:OE2	2.19	0.43
1:B:687:LEU:HA	1:B:687:LEU:HD23	1.79	0.43
1:C:618:ILE:CD1	1:C:687:LEU:HD23	2.49	0.43
1:C:780:LEU:HD22	1:C:875:VAL:HG21	2.01	0.43
1:B:152:LEU:O	1:B:154:GLU:N	2.52	0.43
1:C:283:ASP:HB2	1:C:290:TYR:CE2	2.54	0.43
1:C:598:ARG:NH1	1:C:653:ASN:HA	2.31	0.43
1:D:426:HIS:CE1	1:D:429:ALA:H	2.37	0.43
1:D:476:ASN:HD22	1:D:503:SER:HB2	1.83	0.43
1:A:115:LEU:HD12	1:A:116:LEU:N	2.34	0.43
1:A:425:TYR:HD1	1:A:461:PRO:HG3	1.84	0.43
1:A:536:GLN:O	1:A:540:ASN:ND2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:THR:HB	1:C:28:SER:HB3	2.01	0.43
1:C:544:ILE:HG22	1:C:598:ARG:HH21	1.84	0.43
1:A:400:LEU:HD23	1:A:439:LEU:HG	2.00	0.42
1:A:500:CYS:HB3	1:A:508:ARG:HH21	1.84	0.42
1:B:853:ASN:O	1:B:854:HIS:ND1	2.52	0.42
1:B:711:TYR:CD1	1:B:723:PRO:HD3	2.54	0.42
1:B:787:TYR:CE1	1:B:877:LYS:HB2	2.54	0.42
1:C:364:GLU:OE2	1:C:367:ARG:NH1	2.52	0.42
1:A:552:ASP:OD1	1:A:552:ASP:N	2.49	0.42
1:C:232:GLU:HB2	1:C:273:TYR:OH	2.19	0.42
1:C:480:VAL:HG21	1:C:496:PHE:CE2	2.55	0.42
1:C:858:GLU:OE1	1:C:860:LEU:HD21	2.19	0.42
1:C:638:GLU:HB2	1:C:648:VAL:CG2	2.46	0.42
1:D:545:ASN:OD1	1:D:598:ARG:NH1	2.45	0.42
1:A:416:TRP:HB2	1:A:440:LYS:HD3	2.01	0.42
1:C:26:GLU:HG2	1:C:176:GLN:HB3	2.01	0.42
1:A:457:THR:HA	1:A:462:TYR:CD2	2.54	0.42
1:B:215:ASN:O	1:B:248:PRO:HA	2.20	0.42
1:C:183:PHE:CE2	1:C:213:LEU:HD11	2.54	0.42
1:C:873:LEU:HD12	1:C:873:LEU:HA	1.77	0.42
1:A:548:GLU:OE2	1:A:556:TYR:OH	2.25	0.42
1:C:300:ARG:HE	1:C:411:PRO:HA	1.84	0.42
1:C:559:TRP:HA	1:C:560:ASN:HA	1.81	0.42
1:C:250:ARG:HB3	1:C:252:TYR:CE2	2.55	0.42
1:C:705:LEU:HA	1:C:724:ASP:OD2	2.20	0.42
1:D:103:VAL:O	1:D:122:ALA:HA	2.20	0.42
1:D:326:ASP:HB3	1:D:332:THR:HG22	2.02	0.42
1:D:537:LEU:HG	1:D:541:ARG:HH11	1.84	0.42
1:D:619:CYS:HB3	1:D:686:LEU:HG	2.02	0.42
1:D:705:LEU:HD23	1:D:705:LEU:HA	1.84	0.42
1:B:562:VAL:HG11	1:B:586:ARG:CZ	2.50	0.42
1:C:220:THR:HG23	1:C:247:ILE:HA	2.01	0.42
1:C:832:ASN:O	1:C:836:SER:HB2	2.20	0.42
1:C:839:GLU:HG3	1:C:840:GLN:HG3	2.02	0.42
1:D:454:HIS:CE1	1:D:456:PHE:HB2	2.55	0.42
1:D:456:PHE:CD2	1:D:456:PHE:N	2.88	0.42
1:B:348:GLU:O	1:B:596:GLN:NE2	2.52	0.42
1:D:527:ARG:NH1	3:D:1023:HOH:O	2.53	0.42
1:A:564:PHE:O	1:A:576:LEU:HD12	2.20	0.41
1:B:298:GLY:N	1:B:411:PRO:HG3	2.35	0.41
1:B:660:VAL:HB	1:B:662:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TRP:CZ3	1:C:82:ARG:HD3	2.55	0.41
1:A:187:PRO:HG2	1:A:188:TYR:CE2	2.56	0.41
1:A:194:ARG:HD3	1:A:194:ARG:N	2.35	0.41
1:A:419:MET:HE1	1:A:433:ALA:HB2	2.02	0.41
1:A:458:TRP:HZ2	1:A:486:GLN:HE21	1.68	0.41
1:B:111:LEU:HD23	1:B:133:ILE:HB	2.02	0.41
1:B:532:THR:HB	1:B:534:GLU:OE1	2.21	0.41
1:C:109:VAL:HG22	1:C:144:VAL:HG13	2.01	0.41
1:B:63:ASN:HA	1:B:66:ASP:HB2	2.02	0.41
1:C:259:GLY:O	1:C:261:ILE:HG13	2.20	0.41
1:D:92:ARG:NH2	1:D:136:VAL:O	2.53	0.41
1:B:32:SER:OG	1:B:32:SER:O	2.31	0.41
1:A:540:ASN:O	1:A:544:ILE:HG12	2.21	0.41
1:B:760:LYS:HB2	1:B:841:THR:HG23	2.02	0.41
1:D:106:LYS:HG3	1:D:120:LEU:CD2	2.51	0.41
1:D:220:THR:CG2	1:D:248:PRO:HD3	2.51	0.41
1:D:353:PHE:HE2	1:D:557:SER:OG	2.02	0.41
1:A:876:LYS:HB2	1:A:876:LYS:HE3	1.78	0.41
1:C:154:GLU:HG3	1:C:389:ASN:ND2	2.34	0.41
1:C:373:GLY:O	1:C:374:LEU:HG	2.20	0.41
1:D:355:ARG:HH12	1:D:512:GLU:HG3	1.86	0.41
1:D:560:ASN:O	1:D:580:GLY:HA2	2.21	0.41
1:D:53:TRP:CZ3	1:D:82:ARG:HD3	2.56	0.41
1:A:694:SER:OG	1:A:695:ASP:N	2.53	0.41
1:A:691:LEU:HD13	1:A:782:VAL:HG12	2.03	0.41
1:D:116:LEU:CD1	1:D:130:ILE:HG22	2.50	0.41
1:D:301:TRP:CE2	1:D:312:ASN:HA	2.56	0.41
1:A:434:ARG:HG2	1:A:472:ILE:HD13	2.02	0.41
1:B:251:LYS:HE2	1:B:251:LYS:HB3	1.70	0.41
1:B:451:VAL:HG12	1:B:476:ASN:HA	2.03	0.41
1:C:380:ILE:HG13	1:C:418:ALA:HA	2.02	0.41
1:D:121:GLY:H	1:D:156:LEU:HD21	1.86	0.41
1:C:33:TRP:CD2	1:C:83:LYS:HB2	2.55	0.41
1:C:705:LEU:HD23	1:C:724:ASP:OD2	2.21	0.41
1:B:591:ILE:HA	1:B:591:ILE:HD12	1.80	0.41
1:D:241:GLN:C	1:D:242:LEU:HD23	2.41	0.41
1:C:300:ARG:N	1:C:300:ARG:HD3	2.35	0.41
1:D:323:ARG:CZ	1:D:365:ILE:HD11	2.51	0.41
1:D:66:ASP:O	3:D:1004:HOH:O	2.20	0.41
1:C:466:SER:OG	1:C:467:LYS:N	2.54	0.40
1:D:462:TYR:HD1	1:D:502:TYR:CE2	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:ILE:HD12	1:D:556:TYR:HE2	1.87	0.40
1:A:458:TRP:HD1	1:A:459:GLU:OE1	2.03	0.40
1:B:526:PRO:HG3	1:B:534:GLU:HB3	2.03	0.40
1:B:700:GLY:HA2	1:B:875:VAL:O	2.20	0.40
1:C:302:PHE:CZ	1:C:447:ARG:HA	2.56	0.40
1:D:96:ILE:H	1:D:131:THR:HG23	1.86	0.40
1:D:213:LEU:HD21	1:D:281:VAL:HG21	2.04	0.40
1:A:712:PHE:CE1	1:A:766:PRO:HG2	2.56	0.40
1:B:354:VAL:HG11	1:B:369:CYS:SG	2.61	0.40
1:B:702:CYS:HB3	1:B:721:TRP:CD2	2.56	0.40
1:C:514:GLY:HA3	1:C:559:TRP:O	2.21	0.40
1:D:228:PHE:CD1	1:D:228:PHE:N	2.89	0.40
1:D:695:ASP:OD1	1:D:695:ASP:N	2.48	0.40
1:A:525:THR:OG1	1:A:525:THR:O	2.31	0.40
1:B:304:VAL:O	1:B:304:VAL:HG23	2.20	0.40
1:B:190:ALA:HB2	1:B:405:LEU:HB3	2.03	0.40
1:B:628:ILE:O	1:B:657:VAL:HA	2.22	0.40
1:D:213:LEU:CD1	1:D:254:ILE:HD11	2.51	0.40
1:D:212:PHE:HE1	1:D:253:PRO:HB3	1.86	0.40
1:D:762:THR:HG21	1:D:768:PHE:CD2	2.56	0.40
1:D:876:LYS:HB2	1:D:876:LYS:HE3	1.69	0.40
1:A:507:PRO:HA	1:A:508:ARG:NH1	2.37	0.40
1:A:668:LEU:HD21	1:A:679:ARG:NH2	2.36	0.40
1:B:488:ASP:O	1:B:490:ALA:N	2.54	0.40
1:D:194:ARG:HB3	1:D:408:TYR:CE2	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:OE1	1:D:852:ARG:NH1[1_565]	2.06	0.14
1:A:855:GLU:OE2	1:D:22:SER:OG[1_565]	2.11	0.09

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	858/879 (98%)	783 (91%)	69 (8%)	6 (1%)	24	58
1	B	858/879 (98%)	786 (92%)	63 (7%)	9 (1%)	17	49
1	C	858/879 (98%)	780 (91%)	69 (8%)	9 (1%)	17	49
1	D	858/879 (98%)	771 (90%)	79 (9%)	8 (1%)	19	52
All	All	3432/3516 (98%)	3120 (91%)	280 (8%)	32 (1%)	19	52

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	830	SER
1	B	830	SER
1	C	104	ALA
1	C	105	SER
1	B	32	SER
1	B	219	ASP
1	B	823	ASN
1	C	830	SER
1	A	32	SER
1	A	66	ASP
1	A	709	HIS
1	B	489	SER
1	C	49	ASN
1	C	356	ILE
1	C	586	ARG
1	D	138	LYS
1	D	424	ASP
1	D	571	ASP
1	B	66	ASP
1	B	571	ASP
1	C	32	SER
1	C	571	ASP
1	D	272	PRO
1	D	388	LYS
1	D	553	TYR
1	A	162	ASP
1	B	492	ILE
1	B	674	GLY
1	C	285	LYS
1	D	418	ALA

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Mol	Chain	Res	Type
1	A	544	ILE
1	D	356	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	750/775 (97%)	717 (96%)	33 (4%)	31	65
1	B	752/775 (97%)	727 (97%)	25 (3%)	41	75
1	C	752/775 (97%)	731 (97%)	21 (3%)	47	80
1	D	739/775 (95%)	717 (97%)	22 (3%)	44	78
All	All	2993/3100 (96%)	2892 (97%)	101 (3%)	40	74

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PHE
1	A	41	GLU
1	A	45	SER
1	A	47	ASP
1	A	51	SER
1	A	72	ARG
1	A	141	LEU
1	A	194	ARG
1	A	241	GLN
1	A	245	LYS
1	A	255	SER
1	A	257	SER
1	A	285	LYS
1	A	295	SER
1	A	300	ARG
1	A	347	LYS
1	A	377	TRP
1	A	449	SER
1	A	469	MET

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Mol	Chain	Res	Type
1	A	508	ARG
1	A	529	PHE
1	A	557	SER
1	A	604	MET
1	A	622	SER
1	A	635	LYS
1	A	649	ARG
1	A	655	GLU
1	A	670	ASP
1	A	725	LYS
1	A	800	ASP
1	A	811	SER
1	A	819	ASP
1	A	829	ASP
1	B	28	SER
1	B	47	ASP
1	B	66	ASP
1	B	117	LYS
1	B	219	ASP
1	B	270	GLU
1	B	295	SER
1	B	300	ARG
1	B	340	ARG
1	B	377	TRP
1	B	385	GLU
1	B	508	ARG
1	B	529	PHE
1	B	538	ASP
1	B	552	ASP
1	B	615	ARG
1	B	658	PHE
1	B	668	LEU
1	B	677	SER
1	B	743	TRP
1	B	746	SER
1	B	779	ARG
1	B	800	ASP
1	B	819	ASP
1	B	832	ASN
1	C	36	LYS
1	C	66	ASP
1	C	72	ARG

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Mol	Chain	Res	Type
1	C	92	ARG
1	C	150	SER
1	C	235	ARG
1	C	250	ARG
1	C	300	ARG
1	C	377	TRP
1	C	385	GLU
1	C	469	MET
1	C	508	ARG
1	C	529	PHE
1	C	538	ASP
1	C	549	LYS
1	C	557	SER
1	C	699	ASP
1	C	780	LEU
1	C	799	LYS
1	C	800	ASP
1	C	819	ASP
1	D	106	LYS
1	D	139	GLU
1	D	199	GLU
1	D	228	PHE
1	D	244	LEU
1	D	278	LYS
1	D	300	ARG
1	D	311	LEU
1	D	324	HIS
1	D	341	ARG
1	D	377	TRP
1	D	426	HIS
1	D	449	SER
1	D	469	MET
1	D	471	SER
1	D	483	SER
1	D	506	LYS
1	D	511	SER
1	D	529	PHE
1	D	601	ASP
1	D	677	SER
1	D	829	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	575	ASN
1	D	215	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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

6.1 Protein, DNA and RNA chains

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	860/879 (97%)	-0.39	5 (0%) 89 89	11, 27, 44, 65	0
1	B	860/879 (97%)	-0.44	2 (0%) 94 95	11, 23, 41, 57	0
1	C	860/879 (97%)	-0.35	3 (0%) 93 94	14, 27, 48, 61	0
1	D	860/879 (97%)	-0.16	19 (2%) 62 59	15, 33, 59, 77	0
All	All	3440/3516 (97%)	-0.34	29 (0%) 86 85	11, 27, 51, 77	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	465	SER	3.0
1	D	72	ARG	3.0
1	D	218	THR	3.0
1	C	66	ASP	2.8
1	D	263	ASN	2.8
1	D	66	ASP	2.7
1	B	694	SER	2.7
1	D	463	THR	2.6
1	D	93	ASP	2.5
1	D	287	GLY	2.5
1	D	284	ALA	2.5
1	D	692	THR	2.3
1	D	313	GLY	2.3
1	D	286	ASN	2.3
1	A	623	ILE	2.3
1	D	71	GLN	2.2
1	D	803	LYS	2.2
1	D	602	ILE	2.2
1	D	255	SER	2.2
1	D	70	GLU	2.1
1	A	694	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	675	ALA	2.1
1	D	288	GLU	2.1
1	C	72	ARG	2.1
1	A	51	SER	2.1
1	B	621	ASP	2.0
1	A	219	ASP	2.0
1	A	693	ASP	2.0
1	C	557	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	A	901	1/1	0.88	0.12	27,27,27,27	0
2	NA	C	901	1/1	0.89	0.15	21,21,21,21	0
2	NA	D	901	1/1	0.91	0.13	17,17,17,17	0
2	NA	B	901	1/1	0.99	0.17	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.