



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 1, 2017 – 11:45 PM EDT

PDB ID : 5VHW  
EMDB ID: : EMD-8685  
Title : GluA2-0xGSG1L bound to ZK  
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.  
Deposited on : unknown  
Resolution : 7.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

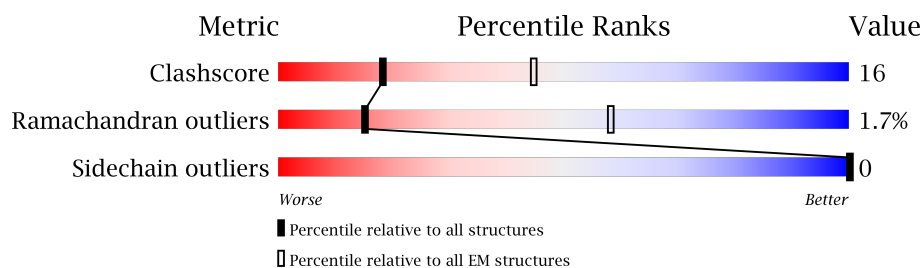
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.80 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1057	
1	B	1057	
1	C	1057	
1	D	1057	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glutamate receptor 2,Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	B	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	C	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	D	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		

There are 56 discrepancies between the modelled and reference sequences:

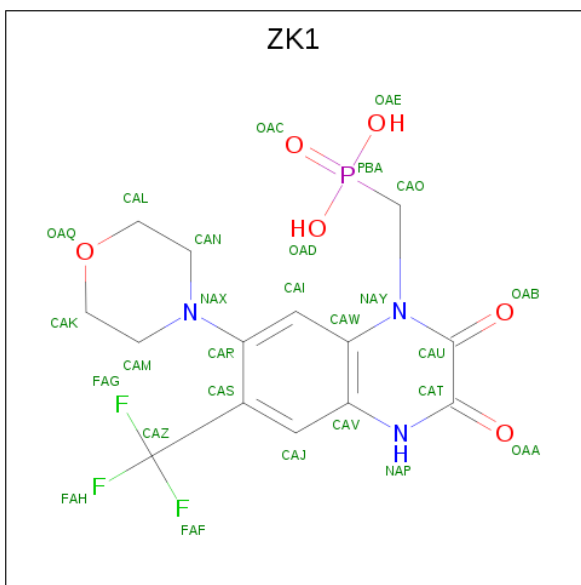
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491

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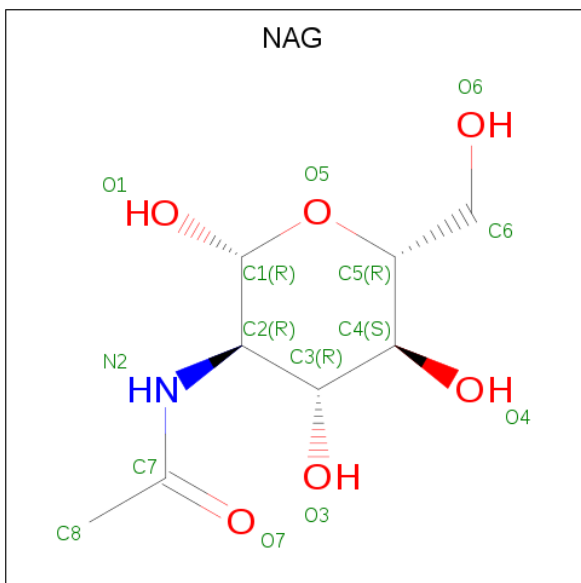
Chain	Residue	Modelled	Actual	Comment	Reference
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C<sub>14</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	







R114	L209	Q324	L415	Q587	Y702	ALA	ASN	ILE	GLY	THR
P115	T210	Q325	N418	G588	L703	LYS	SER	ASP	LEU	VAL
D116	I211	G326	E419	C589	L704	ARG	GLY	LEU	LEU	ILE
L117	G212	V327	E420	D590	E705	MET	ASN	PRO	GLY	GLU
K118	K213	E330	Y421	S592	E708	GLY	ASN	ALA	ALA	PHE
L121	H214	E331	E422	F593	M709	THR	THR	SER	ALA	
L124	Y218	L333	Q425	R594	E710	GLY	ALA	GLY	HIS	
Y128	H219	K334	Q426	S595	E711	GLY	ASN	LEU	MET	
D129	G226	V335	L428	L596	I712	THR	SER	VAL	THR	
H130	F227	Q337	I432	G598	K716	ARG	ALA	THR	THR	
D131	L232	N344	G437	R599	E722	GLY	PRO	LEU	VAL	
K132	Q236	I345	Y440	I600	L727	ALA	VAL	SER	GLN	
A134	E241	I346	Y441	V601	L734	LEU	ALA	LEU	PHE	
D138	Q244	K352	G451	F607	A735	ALA	PRO	ASP	SER	
S139	F245	R353	A452	I611	I736	VAL	ALA	VAL	THR	
L143	Q246	K354	K458	I612	P737	LEU	GLY	LEU	THR	
Q147	V248	N355	K459	I613	E744	ALA	ALA	GLY	THR	
L150	I249	V356	W460	N619	P745	LEU	THR	LEU	THR	
A153	Y250	L363	V464	T625	I746	LEU	TRP	LEU	THR	
V158	V255	K364	G465	R628	N747	LEU	GLU	VAL	THR	
Q159	I259	T365	E466	I633	L748	LEU	ALA	VAL	THR	
V160	V262	P368	L467	E637	E755	THR	ASP	THR	THR	
N169	S263	K369	A472	D638	K763	THR	ARG	LEU	THR	
K172	E267	L371	D473	K641	N764	ALA	PHE	THR	THR	
K173	E268	V373	I474	K642	K765	GLN	GLN	THR	THR	
D174	E269	K374	I476	Q642	K766	LEU	LEU	THR	THR	
Y177	Y270	S375	A477	I645	E772	THR	ARG	THR	THR	
K178	P271	E376	L478	L649	C773	THR	THR	THR	THR	
S179	G272	D378	L490	D651	G774	GLN	GLY	THR	THR	
L180	H274	T387	R485	S652	D777	THR	THR	THR	THR	
D183	D287	K388	K493	F659	L787	GLN	THR	THR	THR	
E185	V291	L390	I500	R660	S788	ARG	SER	THR	THR	
K188	R297	T394	K511	R661	L789	VAL	CYS	THR	THR	
E189	S307	V395	P512	I664	A793	PRO	GLY	THR	THR	
R190	R308	V396	G513	F667	G794	GLY	LEU	THR	THR	
R191	V192	E402	V514	V576	V809	CYS	GLY	THR	THR	
E197	A312	Y405	F515	L577	I812	GLY	GLY	THR	THR	
V201	G313	V406	P520	N575	E813	GLY	GLY	THR	THR	
L204	C315	I521	A522	S580	F814	GLY	GLY	THR	THR	
W323	P322	M407	Y523	L581	K817	ALA	CYS	THR	THR	
		K409	E524	F584	A820	ASN	ARG	THR	THR	
			I525	Q586		SER	SER	THR	THR	

- Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein

Chain D:  45% 28% 26%

N10	F109	I204	L299
S11	Q112	V205	L306
I12	M113	D206	S307
Q13	P114	Q207	R308
G14	R115	V208	R309
G16	D116	I209	G310
Q24	L117	T210	N311
E25	K118	G212	K323
Y26	L122	H214	G324
S27	S123	V215	Q325
V31	I124	G326	T329
Q35	E126	Y218	E330
F41	Y127	H219	R331
R42	Y128	I221	A332
L43	K130	L225	L333
T44	D131	G226	K334
L50	K132	F227	Q335
E51	F133	A134	V336
V52	Y135	D231	L341
A53	R141	L232	N344
N54	G142	L233	T345
F56	L143	K234	K346
A57	F56	Q236	F347
N60	L146	F237	D348
A61	Q147	G238	K349
Q65	A148	E241	N350
Y71	V149	Y242	G351
A72	S152	S243	K352
F76	K156	G244	R353
D78	T161	F245	I354
Y77	A162	Q246	N355
K79	I163	L247	E362
K80	N164	V248	L363
S81	V165	D249	K364
V82	K174	Y250	G372
N83	Y177	V255	T373
S95	R178	T259	K374
T98	K187	E260	S375
P99	R190	R261	E376
S100	R191	W262	V377
F101	I193	S263	D378
P102	C196	T264	T383
G105	E197	H274	T394
H107	V201	T277	V395
P108		I278	V396
		K279	V397
		Y286	T398
		D287	E402

SER	GLU	ARG	THR	THR	E772	T649	ASN	P478	S403
PHE	LEU	ARG	THR	THR	E776	L690	GLU	L479	P404
CYS	LEU	PHE	TYR	TYR	K776	D651	PHE	T480	Y405
ALA	SER	HIS	TRP	TRP	E782	V666	GLY	I481	V406
TRP	SER	THR	CYS	CYS	E782	V666	THR	R485	N407
GLY	SER	ILE	GLY	GLN	L787	F682	ILE	R408	K409
SER	VAL	TRP	GLY	GLY	L787	V683	S576	F491	K410
VAL	ILE	TRP	THR	THR	L787	V683	S576	S492	N411
PHE	ILE	TRP	GLN	GLN	L789	R694	S577	F491	N411
THR	ASP	SER	ARG	ARG	L789	T685	N578	S492	N412
THR	GLY	SER	VAL	VAL	S790	T685	F579	P494	N413
CYS	GLY	CYS	VAL	VAL	S790	T685	F579	P494	N413
GLY	LEU	GLY	PRO	PRO	N791	E688	S580	K505	N414
VAL	LYS	GLY	LYS	LYS	N792	V792	L581	K505	N414
LEU	GLY	GLY	PRO	PRO	V792	R682	G582	K505	N414
LEU	GLY	GLY	GLY	GLY	F796	S696	G583	P512	E419
ASN	ASN	GLY	GLY	GLY	V800	K697	Q586	G513	E422
ALA	ALA	PRO	GLY	GLY	V800	K697	Q587	V514	E422
SER	PHE	PRO	GLY	GLY	L803	Y700	G588	F515	Q425
THR	ALA	GLY	GLY	GLY	L803	Y700	G588	F515	Q425
LEU	VAL	GLY	GLY	GLY	P817	A701	C589	P620	N427
ASN	PHE	LYS	LYS	LYS	P817	Y702	D590	L521	N428
THR	THR	CYS	ALA	ALA	P817	L703	S591	A522	E431
LYS	LEU	ARG	ALA	ALA	P817	L704	S592	Y523	E431
THR	THR	ASN	ALA	ALA	P817	E705	P593	K526	I432
LYS	SER	PRO	PRO	PRO	P817	Y708	R594	K526	I432
THR	GLY	ILE	ASN	ASN	P817	Y708	S595	K435	K435
VAL	LEU	ASP	SER	SER	P817	N709	L596	C436	C436
ILE	LEU	LEU	GLY	GLY	P817	E710	S597	G437	G437
VAL	LEU	LEU	GLY	GLY	P817	Y711	G598	F438	F438
GLY	GLY	ALA	ALA	ALA	P817	I712	R599	K439	K439
THR	THR	PRO	ALA	ALA	P817	I713	T600	V336	V336
THR	ALA	ALA	ALA	ALA	P817	Q714	T601	S837	L442
GLY	GLY	GLY	ALA	ALA	P817	R715	G602	T443	T443
LYS	LYS	LYS	ALA	ALA	P817	K716	G603	V444	V444
THR	THR	THR	THR	THR	P817	T720	K606	S544	S544
THR	THR	THR	THR	THR	P817	Y721	F607	ARG	G451
THR	THR	THR	THR	THR	P817	K722	F608	PHE	A452
THR	THR	THR	THR	THR	P817	K722	F608	SER	R453
THR	THR	THR	THR	THR	P817	K722	F608	PRO	D454
THR	THR	THR	THR	THR	P817	K722	F608	TYR	K458
THR	THR	THR	THR	THR	P817	K722	F608	TRP	I459
THR	THR	THR	THR	THR	P817	K722	F608	HIS	N460
THR	THR	THR	THR	THR	P817	K722	F608	THR	N461
THR	THR	THR	THR	THR	P817	K722	F608	GLU	G462
THR	THR	THR	THR	THR	P817	K722	F608	GLU	N463
THR	THR	THR	THR	THR	P817	K722	F608	PHE	V464
THR	THR	THR	THR	THR	P817	K722	F608	GLY	G465
THR	THR	THR	THR	THR	P817	K722	F608	ASP	E466
THR	THR	THR	THR	THR	P817	K722	F608	GLY	L467
THR	THR	THR	THR	THR	P817	K722	F608	ARG	V468
THR	THR	THR	THR	THR	P817	K722	F608	THR	K471
THR	THR	THR	THR	THR	P817	K722	F608	GLN	A472
THR	THR	THR	THR	THR	P817	K722	F608	SER	D473
THR	THR	THR	THR	THR	P817	K722	F608	SER	I474
THR	THR	THR	THR	THR	P817	K722	F608	GLU	A475
THR	THR	THR	THR	THR	P817	K722	F608	SER	I476
THR	THR	THR	THR	THR	P817	K722	F608	THR	A477
THR	THR	THR	THR	THR	P817	K722	F608	THR	A477

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	14372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 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: NAG, ZK1

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.33	0/6287	0.46	0/8493
1	B	0.32	0/6265	0.45	0/8464
1	C	0.32	0/6287	0.45	0/8493
1	D	0.32	0/6265	0.45	0/8464
All	All	0.32	0/25104	0.45	0/33914

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	6159	0	6155	216	0
1	B	6137	0	6132	217	0
1	C	6159	0	6155	214	0
1	D	6137	0	6132	234	0
2	A	27	0	13	4	0
2	B	27	0	13	2	0
2	C	27	0	13	3	0
2	D	27	0	13	2	0
3	A	14	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
3	C	14	0	13	2	0
3	D	14	0	13	3	0
All	All	24756	0	24678	814	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 16.

All (814) 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:C:337:GLN:HG3	1:C:346:LYS:HG2	1.58	0.82
1:B:595:SER:HA	1:B:599:ARG:HB2	1.63	0.81
1:A:190:ARG:HE	1:A:469:TYR:HB3	1.46	0.81
1:A:188:LYS:HD2	1:A:190:ARG:HH22	1.46	0.80
1:B:209:ILE:HA	1:B:214:HIS:HD2	1.46	0.80
1:D:247:ILE:HG23	1:D:248:VAL:HG23	1.64	0.80
1:D:595:SER:HA	1:D:599:ARG:HB3	1.64	0.78
1:A:77:TYR:HE2	1:A:98:THR:HG21	1.49	0.77
1:B:246:GLN:HE21	1:B:248:VAL:H	1.33	0.76
1:C:77:TYR:HE2	1:C:98:THR:HG21	1.51	0.75
1:D:308:ARG:NH2	1:D:325:GLN:OE1	2.19	0.75
1:A:451:GLY:O	1:A:485:ARG:NH2	2.20	0.74
1:C:344:ASN:HD21	1:C:346:LYS:HE3	1.51	0.74
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.69	0.74
1:A:475:ALA:HB3	1:A:735:ALA:HB3	1.69	0.73
1:B:247:ILE:HG23	1:B:248:VAL:HG23	1.69	0.73
1:D:523:TYR:HA	1:D:526:TRP:HD1	1.52	0.73
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.70	0.72
1:A:600:ILE:HA	1:B:581:LEU:HD21	1.71	0.72
1:C:475:ALA:HB3	1:C:735:ALA:HB3	1.69	0.71
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.72	0.71
1:B:16:GLY:H	1:B:65:GLN:HE22	1.38	0.71
1:A:661:ARG:NH1	1:D:755:GLU:O	2.23	0.71
1:D:77:TYR:OH	1:D:101:PHE:O	2.09	0.70
1:D:246:GLN:HE21	1:D:248:VAL:H	1.38	0.70
1:C:599:ARG:NH1	1:D:578:TRP:O	2.24	0.70
1:B:375:SER:HB3	1:B:378:ASP:HB2	1.74	0.70
1:C:451:GLY:O	1:C:485:ARG:NH2	2.22	0.70
1:D:355:ASN:N	1:D:376:GLU:OE2	2.19	0.70
1:B:209:ILE:HA	1:B:214:HIS:CD2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:ILE:HA	1:D:581:LEU:HD21	1.73	0.70
1:D:592:SER:HB3	1:D:599:ARG:HB2	1.73	0.70
1:B:523:TYR:HA	1:B:526:TRP:HD1	1.57	0.69
1:D:16:GLY:H	1:D:65:GLN:HE22	1.40	0.69
1:C:13:GLN:HB3	1:C:70:VAL:HG12	1.75	0.69
1:A:246:GLN:HE21	1:A:248:VAL:H	1.41	0.69
1:B:376:GLU:HG2	1:B:377:VAL:HG13	1.73	0.69
1:A:355:ASN:ND2	3:A:1102:NAG:O6	2.26	0.69
1:A:147:GLN:HE21	1:B:143:LEU:HD21	1.58	0.69
1:D:590:ASP:O	1:D:592:SER:N	2.23	0.69
1:B:77:TYR:OH	1:B:101:PHE:O	2.06	0.68
1:D:592:SER:O	1:D:599:ARG:NH2	2.26	0.68
1:A:586:GLN:HA	1:D:587:GLN:HE21	1.57	0.68
1:A:512:PRO:HB2	1:A:516:SER:HB3	1.74	0.68
1:A:236:GLN:NE2	1:A:365:THR:O	2.26	0.68
1:B:193:ILE:HG12	1:B:221:ILE:HB	1.76	0.68
1:B:579:PHE:HZ	1:B:590:ASP:H	1.41	0.68
1:C:307:SER:O	1:C:308:ARG:NH1	2.25	0.68
1:D:193:ILE:HG12	1:D:221:ILE:HB	1.75	0.67
1:D:537:SER:O	1:D:576:SER:OG	2.12	0.67
1:D:309:ARG:HG2	1:D:311:ASN:H	1.57	0.67
1:B:308:ARG:HH21	1:B:325:GLN:H	1.42	0.67
1:B:346:LYS:HD3	1:B:355:ASN:HD22	1.60	0.67
1:D:716:LYS:HG3	1:D:772:GLU:HB3	1.76	0.67
1:A:11:SER:OG	1:A:44:THR:OG1	2.12	0.67
1:B:692:ARG:O	1:B:696:SER:OG	2.12	0.67
1:B:628:ARG:HG2	1:C:628:ARG:HH12	1.59	0.67
1:D:24:GLN:HE21	1:D:278:ILE:HG13	1.60	0.67
1:A:263:SER:O	1:A:274:HIS:ND1	2.28	0.66
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.77	0.66
1:B:537:SER:O	1:B:576:SER:OG	2.12	0.66
1:B:24:GLN:HE21	1:B:278:ILE:HG13	1.60	0.66
1:A:525:ILE:HG12	1:B:789:LEU:HD13	1.78	0.66
1:C:147:GLN:HE21	1:D:143:LEU:HD21	1.60	0.66
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.76	0.66
1:D:78:ASP:OD1	1:D:79:LYS:N	2.29	0.66
1:A:716:LYS:N	1:A:772:GLU:OE1	2.28	0.65
1:C:716:LYS:N	1:C:772:GLU:OE1	2.29	0.65
1:A:375:SER:HB3	1:A:378:ASP:HB2	1.78	0.65
1:D:583:ALA:HA	1:D:589:CYS:H	1.61	0.65
1:D:51:GLU:HG3	1:D:53:ALA:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:TYR:HA	1:A:526:TRP:HD1	1.60	0.65
1:C:375:SER:HB3	1:C:378:ASP:HB2	1.77	0.65
1:C:592:SER:HB3	1:C:599:ARG:HD3	1.78	0.65
1:D:427:ASP:OD2	1:D:766:TRP:NE1	2.29	0.65
1:A:143:LEU:HD21	1:B:147:GLN:HE21	1.62	0.65
1:B:78:ASP:OD1	1:B:79:LYS:N	2.30	0.65
1:D:579:PHE:HZ	1:D:590:ASP:H	1.44	0.65
1:C:337:GLN:HE21	1:C:346:LYS:HE2	1.63	0.64
1:B:305:GLU:O	1:B:325:GLN:NE2	2.30	0.64
1:B:309:ARG:HG2	1:B:311:ASN:H	1.60	0.64
1:C:143:LEU:HD21	1:D:147:GLN:HE21	1.61	0.64
1:C:259:ILE:HA	1:C:262:TRP:HB3	1.79	0.64
1:C:633:ILE:HG23	1:C:638:ASP:HB2	1.79	0.64
1:B:427:ASP:OD2	1:B:766:TRP:NE1	2.30	0.64
1:D:348:ASP:OD1	1:D:352:LYS:N	2.30	0.64
1:B:716:LYS:HG3	1:B:772:GLU:HB3	1.80	0.64
1:C:78:ASP:OD1	1:C:79:LYS:N	2.31	0.64
1:C:476:ILE:HG12	1:C:734:ILE:HD12	1.78	0.64
1:D:372:GLY:HA2	1:D:383:THR:HG23	1.77	0.64
1:C:520:PRO:O	1:C:619:ASN:ND2	2.31	0.64
1:B:263:SER:O	1:B:274:HIS:ND1	2.28	0.63
1:D:134:ALA:HB3	1:D:192:VAL:HG22	1.80	0.63
1:C:263:SER:O	1:C:274:HIS:ND1	2.31	0.63
1:D:375:SER:HB3	1:D:378:ASP:HB2	1.78	0.63
1:C:539:VAL:HA	1:C:542:LEU:HD12	1.80	0.63
1:C:246:GLN:HE21	1:C:248:VAL:H	1.45	0.63
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.80	0.63
1:B:13:GLN:HA	1:B:44:THR:HB	1.80	0.62
1:C:355:ASN:HD21	3:C:1102:NAG:H4	1.64	0.62
1:A:13:GLN:HB3	1:A:70:VAL:HG12	1.80	0.62
1:B:334:LYS:NZ	1:B:349:GLN:O	2.21	0.62
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.80	0.62
1:B:228:THR:OG1	1:B:246:GLN:OE1	2.15	0.62
1:C:334:LYS:HD3	1:C:349:GLN:HA	1.81	0.62
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.34	0.62
1:A:628:ARG:NH1	1:D:622:ALA:O	2.33	0.62
1:A:623:PHE:HE1	1:B:785:SER:HB2	1.65	0.62
1:A:307:SER:O	1:A:308:ARG:NH1	2.29	0.62
1:A:476:ILE:HG12	1:A:734:ILE:HD12	1.81	0.62
1:C:347:PHE:HE1	1:C:353:ARG:HG2	1.65	0.62
1:D:13:GLN:HA	1:D:44:THR:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:THR:O	1:D:485:ARG:NH1	2.32	0.62
1:C:590:ASP:O	1:C:592:SER:N	2.26	0.62
1:C:594:ARG:HB3	1:D:578:TRP:HE3	1.65	0.62
1:B:134:ALA:HB3	1:B:192:VAL:HG22	1.80	0.62
1:C:11:SER:OG	1:C:44:THR:OG1	2.17	0.62
1:D:164:ASN:OD1	1:D:165:VAL:N	2.33	0.62
1:A:130:TRP:CD2	1:A:191:ARG:HD3	2.34	0.62
1:A:514:VAL:HA	1:A:794:GLY:HA3	1.82	0.62
1:B:348:ASP:OD1	1:B:352:LYS:N	2.32	0.61
1:C:493:LYS:HG2	1:C:747:ASN:HD21	1.65	0.61
1:C:527:MET:O	1:C:531:PHE:CD1	2.53	0.61
1:A:334:LYS:HD3	1:A:349:GLN:HA	1.81	0.61
1:B:35:GLN:OE1	1:B:261:ARG:NH2	2.34	0.61
1:B:520:PRO:O	1:B:619:ASN:ND2	2.33	0.61
1:B:164:ASN:OD1	1:B:165:VAL:N	2.33	0.61
1:B:600:ILE:HG22	1:C:581:LEU:HD11	1.82	0.61
1:D:692:ARG:O	1:D:696:SER:OG	2.11	0.61
1:B:493:LYS:HD3	1:C:493:LYS:HD3	1.82	0.61
1:C:262:TRP:CZ2	1:C:273:ALA:HA	2.36	0.61
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.83	0.61
1:B:436:CYS:HB2	1:B:438:PHE:HE2	1.66	0.61
1:B:250:TYR:HA	1:B:255:VAL:HG11	1.83	0.60
1:A:493:LYS:HD3	1:D:493:LYS:HD3	1.82	0.60
1:D:411:ASN:HB2	1:D:414:MET:HB2	1.84	0.60
1:B:372:GLY:HA2	1:B:383:THR:HG23	1.83	0.60
1:A:50:LEU:HD23	1:A:57:ALA:HB1	1.82	0.60
1:A:308:ARG:HB3	1:A:311:ASN:HD22	1.67	0.60
1:A:355:ASN:N	1:A:376:GLU:OE2	2.25	0.60
1:D:513:GLY:O	1:D:515:PHE:N	2.35	0.60
1:A:78:ASP:OD1	1:A:79:LYS:N	2.34	0.60
1:C:308:ARG:HB3	1:C:311:ASN:HD22	1.66	0.60
1:C:50:LEU:HD23	1:C:57:ALA:HB1	1.84	0.60
1:D:161:THR:OG1	1:D:187:LYS:NZ	2.35	0.60
1:B:25:GLU:HG2	1:B:76:PHE:HZ	1.67	0.59
1:A:266:GLU:HG2	1:A:268:LYS:H	1.67	0.59
1:C:236:GLN:NE2	1:C:365:THR:O	2.34	0.59
1:D:263:SER:O	1:D:274:HIS:ND1	2.31	0.59
1:B:705:GLU:OE1	2:B:1101:ZK1:FAF	2.09	0.59
1:B:483:LEU:N	1:C:755:GLU:OE2	2.30	0.59
1:A:209:ILE:HA	1:A:214:HIS:HD2	1.67	0.59
1:A:539:VAL:HA	1:A:542:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:VAL:N	1:B:473:ASP:OD2	2.34	0.59
1:C:130:TRP:CD2	1:C:191:ARG:HD3	2.37	0.59
1:C:38:THR:HG21	1:C:297:ARG:HH21	1.68	0.59
1:D:593:PRO:HD2	1:D:596:LEU:HD23	1.85	0.59
1:A:787:LEU:HD12	1:D:521:LEU:HA	1.85	0.58
1:D:705:GLU:OE1	2:D:1101:ZK1:FAF	2.11	0.58
1:A:396:VAL:HB	1:A:473:ASP:H	1.67	0.58
1:B:261:ARG:O	1:B:264:THR:OG1	2.18	0.58
1:A:593:PRO:HD2	1:A:596:LEU:HD22	1.85	0.58
1:D:344:ASN:HD22	3:D:1102:NAG:H4	1.69	0.58
1:A:415:LEU:HD13	1:A:419:GLU:HB3	1.85	0.58
1:A:520:PRO:O	1:A:619:ASN:ND2	2.36	0.58
1:C:396:VAL:HB	1:C:473:ASP:H	1.69	0.58
1:D:586:GLN:O	1:D:588:GLY:N	2.36	0.58
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.86	0.58
1:B:579:PHE:HZ	1:B:590:ASP:N	2.00	0.58
1:D:152:SER:O	1:D:156:LYS:N	2.35	0.58
1:D:225:LEU:HD22	1:D:247:ILE:HB	1.85	0.58
1:D:711:TYR:HB2	1:D:767:TRP:HE1	1.68	0.58
1:A:25:GLU:N	1:A:25:GLU:OE1	2.36	0.58
1:A:493:LYS:HG2	1:A:747:ASN:HD21	1.68	0.58
1:C:13:GLN:HA	1:C:44:THR:HB	1.85	0.58
1:C:523:TYR:HA	1:C:526:TRP:HD1	1.68	0.58
1:A:16:GLY:H	1:A:65:GLN:HE22	1.50	0.58
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.86	0.58
1:D:684:ARG:N	1:D:688:GLU:OE1	2.37	0.58
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.85	0.58
1:D:396:VAL:N	1:D:473:ASP:OD2	2.34	0.57
1:A:109:PHE:HZ	1:A:327:VAL:HG22	1.69	0.57
1:A:347:PHE:HE1	1:A:353:ARG:HG2	1.69	0.57
1:B:225:LEU:HD22	1:B:247:ILE:HB	1.87	0.57
1:C:409:LYS:HG3	1:C:415:LEU:HD12	1.85	0.57
1:C:595:SER:H	1:C:599:ARG:HE	1.53	0.57
1:C:78:ASP:N	1:C:81:SER:OG	2.37	0.57
1:B:246:GLN:HE21	1:B:248:VAL:N	2.01	0.57
1:C:345:ILE:HG12	1:C:353:ARG:NH2	2.20	0.57
1:A:77:TYR:OH	1:A:101:PHE:O	2.16	0.57
1:A:633:ILE:HG23	1:A:638:ASP:HB2	1.86	0.57
1:B:594:ARG:HD3	1:C:579:PHE:HB2	1.87	0.57
1:D:642:GLN:NE2	1:D:645:ILE:HB	2.20	0.57
1:A:78:ASP:N	1:A:81:SER:OG	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:GLU:OE1	1:C:25:GLU:N	2.36	0.57
1:D:25:GLU:HG2	1:D:76:PHE:HZ	1.68	0.57
1:A:247:ILE:HG23	1:A:248:VAL:HG23	1.86	0.56
1:D:710:GLU:OE2	1:D:722:LYS:NZ	2.30	0.56
1:A:262:TRP:CZ2	1:A:273:ALA:HA	2.38	0.56
1:A:774:GLY:N	1:A:777:ASP:OD2	2.37	0.56
1:B:813:GLU:HA	1:B:816:TYR:HD2	1.70	0.56
1:A:206:ASP:HA	1:A:209:ILE:HD12	1.88	0.56
1:B:587:GLN:HE21	1:C:586:GLN:HA	1.70	0.56
1:C:531:PHE:N	1:C:531:PHE:CD1	2.73	0.56
1:A:628:ARG:HH21	1:D:628:ARG:HG2	1.69	0.56
1:B:684:ARG:N	1:B:688:GLU:OE1	2.38	0.56
1:C:112:GLN:HE21	1:C:352:LYS:HA	1.71	0.56
1:C:355:ASN:N	1:C:376:GLU:OE2	2.24	0.56
1:A:172:LYS:O	1:A:174:ASP:N	2.38	0.56
1:C:541:PHE:HB2	1:C:576:SER:HB3	1.86	0.56
1:A:326:GLY:HA2	1:A:329:ILE:HD12	1.87	0.56
1:B:642:GLN:NE2	1:B:645:ILE:HB	2.21	0.56
1:D:540:LEU:HD13	1:D:579:PHE:HD2	1.70	0.56
1:C:211:ILE:HG13	1:C:213:LYS:H	1.69	0.56
1:B:12:ILE:O	1:B:44:THR:N	2.37	0.56
1:B:586:GLN:O	1:B:588:GLY:N	2.38	0.56
1:A:134:ALA:HB3	1:A:192:VAL:HG22	1.87	0.56
1:A:625:THR:HG23	1:D:625:THR:HG21	1.87	0.56
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.41	0.56
1:A:587:GLN:NE2	1:B:587:GLN:OE1	2.39	0.56
1:A:30:ARG:NH1	1:A:269:GLU:O	2.39	0.56
1:A:348:ASP:OD1	1:A:352:LYS:N	2.38	0.56
1:C:513:GLY:O	1:C:516:SER:OG	2.16	0.56
1:D:261:ARG:O	1:D:264:THR:OG1	2.17	0.56
1:B:610:LEU:HD21	1:C:613:ILE:HG21	1.87	0.55
1:D:236:GLN:NE2	1:D:364:LYS:O	2.38	0.55
1:B:198:ARG:NH1	1:B:202:ASN:OD1	2.39	0.55
1:C:774:GLY:N	1:C:777:ASP:OD2	2.38	0.55
1:D:299:LEU:HD23	1:D:306:ILE:HG21	1.87	0.55
1:B:130:TRP:CE2	1:B:191:ARG:HD3	2.42	0.55
1:B:219:HIS:HD2	1:B:241:GLU:HB2	1.70	0.55
1:C:178:ARG:NH1	1:C:211:ILE:HG22	2.22	0.55
1:C:23:ASP:HB3	1:C:271:PRO:HG2	1.89	0.55
1:B:146:LEU:O	1:B:149:VAL:HG22	2.06	0.55
1:B:711:TYR:HB2	1:B:767:TRP:HE1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:714:GLN:HE21	1:D:768:TYR:HA	1.71	0.55
1:D:597:SER:O	1:D:600:ILE:HG12	2.06	0.55
1:A:355:ASN:ND2	3:A:1102:NAG:O5	2.40	0.55
1:D:130:TRP:CE2	1:D:191:ARG:HD3	2.42	0.55
1:A:13:GLN:HA	1:A:44:THR:HB	1.89	0.54
1:A:586:GLN:O	1:A:588:GLY:N	2.40	0.54
1:B:608:PHE:CZ	1:B:612:ILE:HD11	2.43	0.54
1:C:453:ARG:HH21	1:C:458:LYS:HB3	1.73	0.54
1:B:27:SER:HB3	1:B:270:TYR:HB3	1.90	0.54
1:C:514:VAL:HG22	1:C:794:GLY:HA2	1.88	0.54
1:D:146:LEU:O	1:D:149:VAL:HG22	2.08	0.54
1:D:334:LYS:NZ	1:D:349:GLN:O	2.24	0.54
1:A:405:TYR:HB3	1:A:425:CYS:SG	2.48	0.54
1:A:402:GLU:H	1:A:406:VAL:HB	1.73	0.54
1:B:185:GLU:OE2	1:B:213:LYS:NZ	2.37	0.54
1:B:236:GLN:NE2	1:B:364:LYS:O	2.38	0.54
1:D:330:GLU:HA	1:D:333:LEU:HD12	1.90	0.54
1:A:453:ARG:HH21	1:A:458:LYS:HB3	1.72	0.54
1:A:531:PHE:N	1:A:531:PHE:CD1	2.73	0.54
1:D:436:CYS:HB2	1:D:438:PHE:HE2	1.73	0.54
1:C:587:GLN:NE2	1:D:587:GLN:OE1	2.40	0.54
1:D:791:ASN:OD1	1:D:792:VAL:HG23	2.08	0.54
1:D:76:PHE:HE1	1:D:99:PRO:HG2	1.72	0.54
1:A:66:PHE:CZ	1:A:312:ALA:HB1	2.42	0.54
1:A:79:LYS:NZ	1:A:140:ASP:HA	2.23	0.54
1:B:77:TYR:HE2	1:B:98:THR:HG21	1.73	0.54
1:B:328:GLU:OE2	1:B:331:ARG:NH1	2.22	0.54
1:B:592:SER:O	1:B:599:ARG:NH2	2.41	0.54
1:D:219:HIS:HD2	1:D:241:GLU:HB2	1.73	0.54
1:C:402:GLU:O	1:C:406:VAL:N	2.35	0.53
1:C:586:GLN:O	1:C:588:GLY:N	2.41	0.53
1:B:161:THR:OG1	1:B:187:LYS:NZ	2.42	0.53
1:B:594:ARG:O	1:B:596:LEU:N	2.42	0.53
1:C:134:ALA:HB3	1:C:192:VAL:HG22	1.90	0.53
1:D:246:GLN:HE21	1:D:248:VAL:N	2.05	0.53
1:A:330:GLU:HG2	1:A:334:LYS:HE3	1.89	0.53
1:C:66:PHE:CZ	1:C:312:ALA:HB1	2.44	0.53
1:C:402:GLU:H	1:C:406:VAL:HB	1.72	0.53
1:A:577:LEU:O	1:A:580:SER:OG	2.20	0.53
1:B:625:THR:HG21	1:C:625:THR:HG23	1.91	0.53
1:D:711:TYR:O	1:D:715:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:TYR:HB3	1:C:425:CYS:SG	2.49	0.53
1:B:628:ARG:HG2	1:C:628:ARG:NH1	2.24	0.53
1:A:477:ALA:O	1:A:479:LEU:N	2.41	0.53
1:B:20:ARG:NE	1:B:49:ASN:O	2.41	0.53
1:C:15:GLY:HA3	1:C:73:ILE:HA	1.91	0.53
1:C:172:LYS:O	1:C:174:ASP:N	2.42	0.53
1:D:77:TYR:HE2	1:D:98:THR:HG21	1.74	0.53
1:C:642:GLN:NE2	1:C:645:ILE:HB	2.23	0.53
1:B:152:SER:O	1:B:156:LYS:N	2.39	0.53
1:C:291:VAL:HG13	1:C:336:VAL:HG11	1.91	0.53
1:B:453:ARG:HB2	1:B:460:TRP:CD2	2.44	0.52
1:C:477:ALA:O	1:C:479:LEU:N	2.41	0.52
1:A:17:LEU:HB2	1:A:75:GLY:HA3	1.91	0.52
1:A:30:ARG:NH2	1:A:269:GLU:OE2	2.35	0.52
1:A:637:GLU:OE1	1:D:776:LYS:NZ	2.39	0.52
1:A:613:ILE:HG21	1:D:610:LEU:HD21	1.91	0.52
1:D:481:ILE:HD11	1:D:733:GLY:HA3	1.90	0.52
1:B:50:LEU:HD23	1:B:57:ALA:HB1	1.92	0.52
1:D:348:ASP:OD1	1:D:351:GLY:N	2.42	0.52
1:D:637:GLU:O	1:D:640:SER:OG	2.21	0.52
1:A:590:ASP:OD1	1:A:591:ILE:N	2.39	0.52
1:B:696:SER:OG	1:B:700:TYR:HB3	2.08	0.52
1:C:531:PHE:N	1:C:531:PHE:HD1	2.05	0.52
1:A:402:GLU:O	1:A:406:VAL:N	2.34	0.52
1:A:594:ARG:O	1:A:596:LEU:N	2.43	0.52
1:C:12:ILE:O	1:C:44:THR:N	2.43	0.52
1:D:227:PHE:CD1	1:D:244:GLY:HA3	2.43	0.52
1:C:267:GLU:HG3	1:C:271:PRO:HA	1.91	0.52
1:A:595:SER:N	1:A:599:ARG:HE	2.08	0.52
1:B:579:PHE:CZ	1:B:591:ILE:HG22	2.45	0.52
1:C:308:ARG:HB3	1:C:311:ASN:ND2	2.25	0.52
1:C:346:LYS:HD2	1:C:355:ASN:HD22	1.74	0.52
1:A:113:MET:HB3	1:A:284:LEU:HD22	1.90	0.52
1:B:480:THR:O	1:B:485:ARG:NH1	2.40	0.52
1:D:409:LYS:NZ	1:D:419:GLU:OE1	2.43	0.51
1:D:412:HIS:CE1	1:D:413:GLU:HG3	2.44	0.51
1:D:529:ILE:HD12	1:D:612:ILE:HD13	1.92	0.51
1:C:138:ASP:OD1	1:C:139:SER:N	2.43	0.51
1:C:595:SER:N	1:C:599:ARG:HE	2.08	0.51
1:D:345:ILE:HG12	1:D:353:ARG:NH2	2.26	0.51
1:D:405:TYR:HB3	1:D:425:CYS:SG	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:TYR:OH	1:C:101:PHE:O	2.13	0.51
1:C:80:LYS:HA	1:D:83:ASN:ND2	2.25	0.51
1:D:595:SER:O	1:D:597:SER:N	2.43	0.51
1:B:330:GLU:HA	1:B:333:LEU:HD12	1.92	0.51
1:C:637:GLU:O	1:C:641:LYS:HG2	2.09	0.51
1:D:714:GLN:NE2	1:D:768:TYR:HA	2.25	0.51
1:A:14:ILE:HG13	1:A:45:PRO:HA	1.93	0.51
1:B:595:SER:HB3	1:C:578:TRP:CG	2.46	0.51
1:A:362:GLU:O	1:A:369:ARG:N	2.44	0.51
1:B:190:ARG:HD3	1:B:218:TYR:CE1	2.45	0.51
1:B:453:ARG:HA	1:B:460:TRP:HA	1.93	0.51
1:C:330:GLU:HG2	1:C:334:LYS:HE3	1.93	0.51
1:D:642:GLN:HE22	1:D:645:ILE:HB	1.76	0.51
1:B:174:ASP:CG	1:B:178:ARG:HH12	2.14	0.51
1:C:227:PHE:CD1	1:C:244:GLY:HA3	2.46	0.51
1:C:595:SER:H	1:C:599:ARG:HH11	1.59	0.51
1:A:581:LEU:HD21	1:D:600:ILE:HA	1.92	0.51
1:A:584:PHE:CZ	1:D:606:TRP:HZ3	2.29	0.51
1:B:348:ASP:OD1	1:B:351:GLY:N	2.44	0.51
1:C:664:ILE:HB	1:C:667:PHE:HD2	1.76	0.51
1:A:369:ARG:NH1	1:A:387:THR:HG23	2.25	0.50
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.92	0.50
1:C:226:GLY:HA2	1:C:246:GLN:HE22	1.75	0.50
1:D:190:ARG:HD3	1:D:218:TYR:CE1	2.46	0.50
1:A:97:ILE:HG13	1:A:111:ILE:HB	1.93	0.50
1:A:185:GLU:OE2	1:A:213:LYS:NZ	2.38	0.50
1:A:595:SER:H	1:A:599:ARG:HE	1.59	0.50
1:B:177:TYR:CD2	1:B:207:GLN:HG3	2.45	0.50
1:D:608:PHE:CZ	1:D:612:ILE:HD11	2.46	0.50
1:A:642:GLN:NE2	1:A:645:ILE:HB	2.26	0.50
1:B:99:PRO:HA	1:B:113:MET:HB2	1.92	0.50
1:B:219:HIS:CD2	1:B:241:GLU:HB2	2.46	0.50
1:C:389:GLY:O	1:C:391:GLU:N	2.44	0.50
1:D:250:TYR:HA	1:D:255:VAL:HG11	1.92	0.50
1:B:46:HIS:HD2	1:B:68:ARG:NH1	2.09	0.50
1:B:710:GLU:OE2	1:B:722:LYS:NZ	2.31	0.50
1:C:364:LYS:HG3	1:C:369:ARG:NH2	2.26	0.50
1:C:467:LEU:HD22	1:C:737:PRO:HD3	1.94	0.50
1:C:480:THR:N	2:C:1101:ZK1:OAA	2.43	0.50
1:A:83:ASN:ND2	1:B:80:LYS:HA	2.26	0.50
1:C:77:TYR:CE2	1:C:100:SER:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ARG:CZ	1:B:230:GLY:HA2	2.42	0.50
1:B:476:ILE:HG12	1:B:734:ILE:HD12	1.93	0.50
1:D:325:GLN:O	1:D:329:ILE:HG13	2.11	0.50
1:B:436:CYS:HB2	1:B:438:PHE:CE2	2.45	0.50
1:C:594:ARG:HD3	1:D:575:ASN:HB2	1.93	0.50
1:D:309:ARG:HD3	1:D:311:ASN:HB2	1.93	0.50
1:A:597:SER:O	1:A:600:ILE:HG12	2.11	0.49
1:A:308:ARG:HB3	1:A:311:ASN:ND2	2.27	0.49
1:B:345:ILE:HG12	1:B:353:ARG:NH2	2.27	0.49
1:C:169:ASN:HD21	1:C:172:LYS:HE3	1.77	0.49
1:D:800:VAL:HA	1:D:803:LEU:HD12	1.94	0.49
1:B:308:ARG:HE	1:B:323:TRP:HE3	1.60	0.49
1:D:454:ASP:O	1:D:458:LYS:HA	2.12	0.49
1:B:132:LYS:NZ	1:B:189:GLU:OE2	2.46	0.49
1:A:80:LYS:HA	1:B:83:ASN:ND2	2.27	0.49
1:B:232:LEU:HB3	1:B:363:LEU:HD22	1.94	0.49
1:B:794:GLY:HA2	1:B:797:TYR:CD2	2.47	0.49
1:C:705:GLU:OE1	2:C:1101:ZK1:FAF	2.21	0.49
1:A:138:ASP:OD1	1:A:139:SER:N	2.45	0.49
1:A:581:LEU:HD11	1:D:600:ILE:HG22	1.95	0.49
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.52	0.49
1:B:428:LEU:O	1:B:432:ILE:HG12	2.13	0.49
1:B:505:LYS:HG3	1:B:719:ASP:HB2	1.93	0.49
1:B:532:ALA:O	1:B:536:VAL:HG23	2.13	0.49
1:D:453:ARG:HB2	1:D:460:TRP:CD2	2.47	0.49
1:A:112:GLN:NE2	1:A:352:LYS:HG2	2.27	0.49
1:A:38:THR:HG21	1:A:297:ARG:HD3	1.93	0.49
1:A:409:LYS:HG2	1:A:422:GLU:CD	2.32	0.49
1:A:664:ILE:HB	1:A:667:PHE:HD2	1.77	0.49
1:C:93:HIS:HB3	1:C:327:VAL:HG22	1.94	0.49
1:D:10:ASN:O	1:D:42:ARG:N	2.42	0.49
1:A:578:TRP:CG	1:D:595:SER:HB3	2.48	0.49
1:A:23:ASP:HB3	1:A:271:PRO:HG2	1.95	0.49
1:D:219:HIS:CD2	1:D:241:GLU:HB2	2.48	0.49
1:A:296:PHE:HA	1:A:299:LEU:HD13	1.94	0.48
1:A:705:GLU:OE1	2:A:1101:ZK1:FAF	2.21	0.48
1:D:174:ASP:CG	1:D:178:ARG:HH12	2.15	0.48
1:A:188:LYS:HD2	1:A:190:ARG:NH2	2.22	0.48
1:A:657:GLU:HA	1:A:660:ARG:HG2	1.94	0.48
1:C:121:LEU:HA	1:C:245:PHE:CZ	2.48	0.48
1:C:355:ASN:ND2	3:C:1102:NAG:H4	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:PRO:HA	1:D:113:MET:HB2	1.94	0.48
1:A:77:TYR:CE2	1:A:100:SER:HB2	2.49	0.48
1:A:592:SER:HB3	1:A:599:ARG:HD3	1.95	0.48
1:B:411:ASN:HB2	1:B:414:MET:HB2	1.94	0.48
1:C:185:GLU:HA	1:C:188:LYS:HA	1.94	0.48
1:D:540:LEU:HD13	1:D:579:PHE:CD2	2.48	0.48
1:D:536:VAL:O	1:D:540:LEU:HG	2.13	0.48
1:A:236:GLN:HA	1:A:363:LEU:HD21	1.95	0.48
1:A:392:GLN:OE1	1:A:438:PHE:HA	2.13	0.48
1:C:97:ILE:HG13	1:C:111:ILE:HB	1.95	0.48
1:D:594:ARG:O	1:D:596:LEU:N	2.47	0.48
1:A:79:LYS:O	1:A:82:VAL:HG12	2.13	0.48
1:B:76:PHE:HE1	1:B:99:PRO:HG2	1.79	0.48
1:D:243:SER:OG	1:D:362:GLU:HG2	2.13	0.48
1:A:267:GLU:HB2	1:A:274:HIS:HB3	1.96	0.48
1:B:642:GLN:HE22	1:B:645:ILE:HB	1.77	0.48
1:B:800:VAL:HA	1:B:803:LEU:HD12	1.96	0.48
1:B:755:GLU:O	1:C:661:ARG:NH1	2.47	0.48
1:D:396:VAL:O	1:D:473:ASP:HB2	2.14	0.48
1:B:412:HIS:CE1	1:B:413:GLU:HG3	2.48	0.48
1:A:345:ILE:HG12	1:A:353:ARG:NH2	2.28	0.48
1:A:594:ARG:HB3	1:B:578:TRP:HE3	1.79	0.48
1:C:100:SER:C	1:C:114:ARG:HD3	2.34	0.48
2:D:1101:ZK1:HA1	2:D:1101:ZK1:HAOA	1.73	0.48
1:D:355:ASN:ND2	3:D:1102:NAG:O5	2.37	0.48
1:A:383:THR:HG22	1:A:385:ASP:H	1.78	0.48
1:A:651:ASP:HA	1:A:682:PHE:HB3	1.96	0.48
1:B:15:GLY:N	1:B:72:ALA:O	2.40	0.48
1:C:415:LEU:HD13	1:C:419:GLU:HB3	1.96	0.48
1:A:783:LYS:HD3	1:D:630:VAL:HG21	1.94	0.48
1:A:594:ARG:HD3	1:B:575:ASN:HB2	1.94	0.47
1:B:529:ILE:HD12	1:B:612:ILE:HD13	1.96	0.47
1:D:435:HIS:CD2	1:D:753:LEU:HD21	2.49	0.47
1:A:130:TRP:CZ3	1:A:191:ARG:HB3	2.49	0.47
1:A:628:ARG:HH12	1:D:623:PHE:HA	1.79	0.47
1:B:795:VAL:HA	1:B:798:ILE:HG22	1.94	0.47
1:B:347:PHE:HE1	1:B:353:ARG:HG2	1.80	0.47
1:D:696:SER:OG	1:D:700:TYR:HB3	2.13	0.47
1:A:259:ILE:HA	1:A:262:TRP:HB3	1.95	0.47
1:B:526:TRP:HA	1:B:529:ILE:HG22	1.96	0.47
1:D:77:TYR:CE2	1:D:100:SER:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HA	1:A:245:PHE:CZ	2.50	0.47
1:A:459:ILE:HG23	1:A:469:TYR:OH	2.14	0.47
1:A:708:MET:O	1:A:712:ILE:HG12	2.14	0.47
1:A:744:THR:HB	1:A:745:PRO:HD3	1.97	0.47
1:C:363:LEU:HA	1:C:368:PRO:HA	1.95	0.47
1:C:594:ARG:O	1:C:596:LEU:N	2.45	0.47
1:A:101:PHE:HA	1:A:114:ARG:HH11	1.80	0.47
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.50	0.47
1:B:702:TYR:CD2	1:B:704:LEU:HD23	2.49	0.47
1:C:24:GLN:HE21	1:C:262:TRP:HZ2	1.63	0.47
1:C:428:LEU:O	1:C:432:ILE:HG12	2.14	0.47
1:C:532:ALA:O	1:C:536:VAL:HG23	2.15	0.47
1:C:744:THR:HB	1:C:745:PRO:HD3	1.96	0.47
1:D:215:VAL:HA	1:D:238:GLY:O	2.15	0.47
1:B:308:ARG:NE	1:B:323:TRP:HB2	2.29	0.47
1:B:746:VAL:O	1:B:750:VAL:HG23	2.14	0.47
1:C:534:ILE:O	1:C:537:SER:OG	2.23	0.47
1:D:231:ASP:HB3	1:D:234:LYS:HE3	1.97	0.47
1:D:711:TYR:HB2	1:D:767:TRP:NE1	2.30	0.47
1:B:711:TYR:O	1:B:715:ARG:HG2	2.15	0.47
1:C:211:ILE:HD12	1:C:213:LYS:HD2	1.95	0.47
1:C:112:GLN:NE2	1:C:352:LYS:HG2	2.30	0.47
1:A:482:THR:O	1:A:486:GLU:N	2.48	0.47
1:B:397:VAL:HB	1:B:442:LEU:HD23	1.97	0.47
1:B:400:ILE:HG21	1:B:450:TYR:CE1	2.49	0.47
1:B:400:ILE:HG21	1:B:450:TYR:HE1	1.80	0.47
1:B:396:VAL:O	1:B:473:ASP:HB2	2.15	0.47
1:D:116:ASP:OD1	1:D:118:LYS:HG2	2.15	0.47
1:D:453:ARG:HB2	1:D:460:TRP:CE3	2.49	0.47
1:D:744:THR:HB	1:D:745:PRO:HD3	1.97	0.47
1:A:124:LEU:HD11	1:A:128:TYR:HE1	1.80	0.47
1:C:219:HIS:HD2	1:C:241:GLU:OE1	1.98	0.47
1:D:452:ALA:N	1:D:461:ASN:OD1	2.48	0.46
1:B:243:SER:OG	1:B:362:GLU:HG2	2.15	0.46
1:B:325:GLN:O	1:B:329:ILE:HG13	2.14	0.46
1:B:744:THR:HB	1:B:745:PRO:HD3	1.97	0.46
1:C:409:LYS:HG2	1:C:420:ARG:O	2.15	0.46
1:D:12:ILE:O	1:D:44:THR:N	2.42	0.46
1:B:141:ARG:HH22	1:B:196:CYS:N	2.13	0.46
1:B:309:ARG:HD3	1:B:311:ASN:HB2	1.96	0.46
1:C:177:TYR:HE2	1:C:204:ILE:HG12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:ARG:HH22	1:D:581:LEU:C	2.19	0.46
1:D:50:LEU:HD22	1:D:61:ALA:HB2	1.98	0.46
1:C:197:GLU:O	1:C:201:VAL:HG23	2.16	0.46
1:B:266:GLU:HG2	1:B:268:LYS:H	1.80	0.46
1:C:710:GLU:OE2	1:C:722:LYS:NZ	2.48	0.46
1:D:464:VAL:O	1:D:468:VAL:HG23	2.16	0.46
1:A:428:LEU:O	1:A:432:ILE:HG12	2.15	0.46
1:C:323:TRP:CE3	1:C:325:GLN:HB2	2.51	0.46
1:C:522:ALA:H	1:C:525:ILE:HD12	1.79	0.46
1:D:346:LYS:HD3	1:D:355:ASN:HD22	1.79	0.46
1:D:428:LEU:O	1:D:432:ILE:HG12	2.15	0.46
1:D:590:ASP:OD1	1:D:599:ARG:NH2	2.49	0.46
1:B:77:TYR:CE2	1:B:100:SER:HB2	2.51	0.46
1:B:250:TYR:OH	1:B:277:THR:HB	2.16	0.46
1:B:481:ILE:HG12	1:B:491:PHE:CD1	2.50	0.46
1:C:209:ILE:HA	1:C:214:HIS:HD2	1.81	0.46
1:C:330:GLU:HA	1:C:333:LEU:HD12	1.98	0.46
1:C:789:LEU:HG	1:C:793:ALA:HB2	1.98	0.46
1:D:197:GLU:O	1:D:201:VAL:HG23	2.16	0.46
1:D:326:GLY:HA2	1:D:329:ILE:HD12	1.97	0.46
1:A:480:THR:N	2:A:1101:ZK1:OAA	2.42	0.46
1:A:255:VAL:O	1:A:259:ILE:HG12	2.15	0.46
1:B:24:GLN:NE2	1:B:278:ILE:HG13	2.27	0.46
1:A:499:GLY:O	1:A:706:SER:N	2.49	0.46
1:B:15:GLY:HA3	1:B:73:ILE:HA	1.98	0.46
1:B:10:ASN:N	1:B:41:PHE:HA	2.31	0.46
1:B:464:VAL:O	1:B:468:VAL:HG23	2.15	0.46
1:B:637:GLU:O	1:B:640:SER:OG	2.20	0.46
1:D:526:TRP:HA	1:D:529:ILE:HG22	1.98	0.46
1:D:702:TYR:CD2	1:D:704:LEU:HD23	2.51	0.46
1:A:453:ARG:HB2	1:A:460:TRP:CE2	2.51	0.46
1:A:481:ILE:HG12	1:A:491:PHE:CD1	2.51	0.46
1:A:78:ASP:N	1:A:81:SER:HG	2.14	0.46
1:C:227:PHE:N	1:C:246:GLN:OE1	2.49	0.46
1:C:30:ARG:NH2	1:C:269:GLU:OE2	2.46	0.46
1:D:27:SER:O	1:D:31:VAL:HG23	2.16	0.46
1:D:374:TRP:CH2	1:D:376:GLU:HA	2.51	0.46
1:B:651:ASP:HA	1:B:682:PHE:HB3	1.97	0.45
1:B:704:LEU:HD12	1:B:705:GLU:O	2.17	0.45
1:D:204:ILE:O	1:D:208:VAL:HG23	2.16	0.45
1:D:347:PHE:HE1	1:D:353:ARG:HG2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ARG:HH12	1:A:386:ASP:C	2.20	0.45
1:B:427:ASP:O	1:B:431:GLU:HG2	2.16	0.45
1:A:595:SER:HB2	1:B:578:TRP:CG	2.51	0.45
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.81	0.45
2:B:1101:ZK1:HAOA	2:B:1101:ZK1:HAI	1.72	0.45
1:D:481:ILE:HG12	1:D:491:PHE:CD1	2.51	0.45
1:A:628:ARG:NH2	1:D:628:ARG:HG2	2.32	0.45
1:A:540:LEU:HD12	1:A:580:SER:HB3	1.98	0.45
1:A:639:LEU:HA	1:A:642:GLN:HG2	1.98	0.45
1:B:600:ILE:HA	1:C:581:LEU:HD21	1.99	0.45
1:C:124:LEU:HD11	1:C:128:TYR:HE2	1.81	0.45
1:C:153:ALA:HA	1:C:158:TRP:HB2	1.98	0.45
1:D:332:ALA:O	1:D:336:VAL:HG23	2.16	0.45
1:D:746:VAL:O	1:D:750:VAL:HG23	2.15	0.45
1:B:711:TYR:HB2	1:B:767:TRP:NE1	2.31	0.45
1:C:189:GLU:O	1:C:190:ARG:NH1	2.44	0.45
1:C:255:VAL:O	1:C:259:ILE:HG12	2.16	0.45
1:D:250:TYR:OH	1:D:277:THR:HB	2.17	0.45
1:D:397:VAL:HB	1:D:442:LEU:HD23	1.98	0.45
1:B:128:TYR:HB3	1:B:130:TRP:NE1	2.31	0.45
1:B:329:ILE:O	1:B:333:LEU:HG	2.17	0.45
1:C:453:ARG:HB2	1:C:460:TRP:CE2	2.52	0.45
1:A:533:TYR:CE1	1:A:584:PHE:HB2	2.52	0.45
1:B:98:THR:HA	1:B:99:PRO:HD3	1.77	0.45
1:A:453:ARG:HB2	1:A:460:TRP:CD2	2.52	0.45
1:A:526:TRP:HA	1:A:529:ILE:HG22	1.99	0.45
1:C:116:ASP:OD1	1:C:118:LYS:HG2	2.17	0.45
1:D:436:CYS:HB2	1:D:438:PHE:CE2	2.50	0.45
1:B:100:SER:HA	1:B:114:ARG:NH2	2.32	0.45
1:C:348:ASP:OD1	1:C:352:LYS:N	2.49	0.45
1:C:813:GLU:O	1:C:817:LYS:HG3	2.17	0.45
1:A:246:GLN:HE21	1:A:248:VAL:N	2.11	0.45
1:A:296:PHE:CD1	1:A:299:LEU:HD22	2.52	0.45
1:A:502:ILE:O	1:A:722:LYS:HA	2.17	0.45
1:B:297:ARG:O	1:B:301:LYS:HG2	2.17	0.45
1:B:35:GLN:HG2	1:B:286:TYR:OH	2.17	0.45
1:B:453:ARG:HB2	1:B:460:TRP:CE2	2.52	0.45
1:B:657:GLU:HG2	1:B:660:ARG:NH1	2.31	0.45
1:B:648:GLY:HA3	1:B:681:VAL:HB	1.99	0.45
1:B:650:LEU:HD12	1:B:683:VAL:O	2.17	0.45
1:A:628:ARG:NH1	1:D:623:PHE:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASP:OD1	1:B:132:LYS:N	2.49	0.44
1:B:197:GLU:O	1:B:201:VAL:HG23	2.17	0.44
1:D:231:ASP:OD1	1:D:232:LEU:N	2.51	0.44
1:A:607:PHE:O	1:A:611:ILE:HG12	2.18	0.44
1:B:309:ARG:HG2	1:B:311:ASN:N	2.30	0.44
1:D:637:GLU:HG2	1:D:666:VAL:HG21	1.98	0.44
1:D:78:ASP:N	1:D:81:SER:OG	2.50	0.44
1:C:595:SER:N	1:C:599:ARG:HH11	2.15	0.44
1:C:708:MET:O	1:C:712:ILE:HG12	2.17	0.44
1:D:10:ASN:N	1:D:41:PHE:HA	2.32	0.44
1:D:232:LEU:HB3	1:D:363:LEU:HD22	1.99	0.44
1:D:407:MET:N	1:D:422:GLU:O	2.49	0.44
1:D:598:GLY:O	1:D:601:VAL:HB	2.18	0.44
1:D:704:LEU:HD12	1:D:705:GLU:O	2.17	0.44
1:A:500:ILE:HB	1:A:727:LEU:HB2	1.98	0.44
1:B:541:PHE:HB2	1:B:576:SER:HB2	1.99	0.44
1:C:250:TYR:HA	1:C:255:VAL:HG11	1.98	0.44
1:C:267:GLU:CG	1:C:271:PRO:HA	2.48	0.44
1:D:329:ILE:O	1:D:333:LEU:HG	2.18	0.44
1:D:466:GLU:HA	1:D:471:LYS:HB2	1.99	0.44
1:B:52:VAL:HG21	1:B:78:ASP:H	1.83	0.44
1:B:619:ASN:ND2	1:C:787:LEU:HB2	2.33	0.44
1:B:95:SER:HA	1:B:109:PHE:HB3	1.99	0.44
1:C:526:TRP:HA	1:C:529:ILE:HG22	2.00	0.44
1:C:619:ASN:HD22	1:D:787:LEU:HD22	1.82	0.44
1:C:598:GLY:O	1:C:601:VAL:HB	2.18	0.44
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.98	0.44
1:D:99:PRO:O	1:D:114:ARG:HB2	2.17	0.44
1:D:35:GLN:HG2	1:D:286:TYR:OH	2.17	0.44
1:A:314:ASP:OD1	1:A:315:CYS:N	2.51	0.44
1:A:784:THR:OG1	1:A:785:SER:N	2.47	0.44
1:D:403:SER:HA	1:D:404:PRO:HA	1.80	0.44
1:A:664:ILE:HA	1:D:761:LYS:HZ3	1.83	0.44
1:A:201:VAL:O	1:A:205:VAL:HG23	2.18	0.44
1:A:400:ILE:HG12	1:A:402:GLU:HG2	1.99	0.44
1:A:678:GLU:HA	1:A:679:PRO:C	2.38	0.44
1:B:204:ILE:O	1:B:208:VAL:HG23	2.18	0.44
1:B:462:GLY:O	1:B:466:GLU:HG3	2.18	0.44
1:D:532:ALA:O	1:D:536:VAL:HG23	2.18	0.44
1:D:787:LEU:HD11	1:D:791:ASN:HD21	1.83	0.44
1:A:598:GLY:O	1:A:601:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:SER:O	1:B:31:VAL:HG23	2.17	0.44
1:B:481:ILE:HD11	1:B:733:GLY:HA3	1.99	0.44
1:C:130:TRP:CZ3	1:C:191:ARG:HB3	2.53	0.44
1:C:370:LYS:HG2	1:C:372:GLY:H	1.82	0.44
1:D:100:SER:HA	1:D:114:ARG:NH2	2.33	0.44
1:D:592:SER:OG	1:D:595:SER:O	2.28	0.44
1:A:585:MET:HG3	1:D:603:GLY:HA2	2.00	0.44
1:A:219:HIS:HD2	1:A:241:GLU:OE1	2.01	0.43
1:C:26:TYR:CE2	1:C:30:ARG:HD2	2.53	0.43
1:C:453:ARG:HB2	1:C:460:TRP:CD2	2.53	0.43
1:D:130:TRP:CD2	1:D:191:ARG:HD3	2.53	0.43
1:D:227:PHE:CG	1:D:244:GLY:HA3	2.53	0.43
1:C:590:ASP:CG	1:C:591:ILE:H	2.22	0.43
1:D:177:TYR:CD2	1:D:207:GLN:HG3	2.52	0.43
1:D:287:ASP:CG	1:D:341:LEU:H	2.22	0.43
1:D:607:PHE:O	1:D:611:ILE:HG12	2.17	0.43
1:A:813:GLU:O	1:A:817:LYS:HG3	2.18	0.43
1:B:606:TRP:HZ3	1:C:584:PHE:CZ	2.35	0.43
1:B:62:PHE:CE2	1:B:88:PHE:HB3	2.53	0.43
1:D:128:TYR:HB3	1:D:130:TRP:NE1	2.33	0.43
1:D:246:GLN:HG3	1:D:248:VAL:H	1.82	0.43
1:D:402:GLU:O	1:D:405:TYR:N	2.51	0.43
1:C:619:ASN:ND2	1:D:787:LEU:HB2	2.33	0.43
1:A:702:TYR:CE2	1:A:704:LEU:HD23	2.54	0.43
1:C:809:VAL:HA	1:C:812:ILE:HG12	2.00	0.43
1:C:97:ILE:HA	1:C:111:ILE:HB	2.00	0.43
1:D:122:LEU:O	1:D:126:GLU:HG3	2.17	0.43
1:D:685:THR:OG1	1:D:688:GLU:HG3	2.18	0.43
1:A:150:LEU:HD23	1:A:160:VAL:HG21	2.01	0.43
1:A:640:SER:HB2	1:A:669:LYS:HD2	2.01	0.43
1:A:790:SER:HA	1:A:793:ALA:HB3	2.00	0.43
1:B:130:TRP:CD2	1:B:191:ARG:HD3	2.54	0.43
1:D:57:ALA:HA	1:D:60:ASN:ND2	2.33	0.43
1:D:95:SER:HA	1:D:109:PHE:HB3	2.00	0.43
1:A:534:ILE:O	1:A:537:SER:OG	2.24	0.43
1:A:599:ARG:NH1	1:B:578:TRP:O	2.52	0.43
1:D:124:LEU:HD11	1:D:128:TYR:HE1	1.84	0.43
1:D:131:ASP:OD1	1:D:132:LYS:N	2.51	0.43
1:C:525:ILE:HG12	1:D:789:LEU:HB2	2.01	0.43
1:B:262:TRP:CZ2	1:B:273:ALA:HA	2.54	0.43
1:B:348:ASP:OD2	1:B:350:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LYS:O	1:C:82:VAL:HG12	2.19	0.43
1:D:24:GLN:NE2	1:D:278:ILE:HG13	2.29	0.43
1:D:592:SER:OG	1:D:596:LEU:HB3	2.19	0.43
1:B:116:ASP:OD1	1:B:118:LYS:HG2	2.17	0.43
1:B:403:SER:HA	1:B:404:PRO:HA	1.83	0.43
1:B:466:GLU:O	1:B:471:LYS:N	2.52	0.43
1:C:619:ASN:HD21	1:D:787:LEU:HB2	1.83	0.43
1:C:702:TYR:CD2	1:C:704:LEU:HD23	2.54	0.43
1:D:71:TYR:HE1	1:D:308:ARG:HB3	1.84	0.43
1:A:466:GLU:HA	1:A:471:LYS:HB3	2.01	0.43
1:C:113:MET:O	1:C:115:PRO:HD3	2.18	0.43
1:C:180:LEU:O	1:C:183:ASP:HB2	2.18	0.43
1:C:418:ASN:ND2	1:C:440:TYR:O	2.46	0.43
1:C:595:SER:H	1:C:599:ARG:NE	2.15	0.43
1:D:344:ASN:ND2	3:D:1102:NAG:H4	2.31	0.43
1:A:527:MET:O	1:A:531:PHE:CD1	2.71	0.43
1:A:664:ILE:HA	1:D:761:LYS:NZ	2.34	0.43
1:B:172:LYS:O	1:B:174:ASP:N	2.52	0.43
1:B:190:ARG:HA	1:B:218:TYR:CD1	2.54	0.43
1:C:599:ARG:HH22	1:D:582:GLY:N	2.17	0.43
1:D:477:ALA:O	1:D:479:LEU:N	2.51	0.43
1:A:479:LEU:HD12	2:A:1101:ZK1:OAA	2.18	0.42
1:A:197:GLU:O	1:A:201:VAL:HG23	2.18	0.42
1:A:452:ALA:N	1:A:461:ASN:OD1	2.35	0.42
1:A:702:TYR:CD2	1:A:704:LEU:HD23	2.54	0.42
1:B:122:LEU:O	1:B:126:GLU:HG3	2.19	0.42
1:C:763:LYS:HA	1:C:767:TRP:CE3	2.54	0.42
1:A:247:ILE:HG13	1:A:342:SER:HB2	2.01	0.42
1:A:763:LYS:HA	1:A:767:TRP:CE3	2.53	0.42
1:B:215:VAL:HA	1:B:238:GLY:O	2.18	0.42
1:B:287:ASP:CG	1:B:341:LEU:H	2.22	0.42
1:B:120:ALA:HA	1:B:374:TRP:CD1	2.54	0.42
1:B:57:ALA:HA	1:B:60:ASN:ND2	2.34	0.42
1:C:132:LYS:HD3	1:C:159:GLN:OE1	2.19	0.42
1:D:16:GLY:H	1:D:65:GLN:NE2	2.12	0.42
1:D:427:ASP:O	1:D:431:GLU:HG2	2.19	0.42
1:B:24:GLN:NE2	1:B:279:LYS:H	2.17	0.42
1:C:511:LYS:HA	1:C:512:PRO:HD3	1.87	0.42
1:C:54:ASN:O	1:C:58:VAL:HG23	2.20	0.42
1:C:540:LEU:HD12	1:C:580:SER:HB3	2.00	0.42
1:D:592:SER:O	1:D:594:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:O	1:A:58:VAL:HG23	2.19	0.42
1:C:227:PHE:CZ	1:C:232:LEU:HD21	2.54	0.42
1:A:584:PHE:HD1	1:A:605:TRP:HZ2	1.66	0.42
1:A:667:PHE:HE1	1:A:727:LEU:HD13	1.84	0.42
1:A:505:LYS:HD3	1:A:697:LYS:HA	2.01	0.42
1:B:124:LEU:HD11	1:B:128:TYR:HE1	1.85	0.42
1:B:112:GLN:HE21	1:B:352:LYS:HG3	1.84	0.42
1:B:453:ARG:HB2	1:B:460:TRP:CE3	2.54	0.42
1:B:708:MET:O	1:B:712:ILE:HG12	2.20	0.42
1:C:190:ARG:HD3	1:C:218:TYR:CE1	2.55	0.42
1:C:287:ASP:O	1:C:291:VAL:HG23	2.20	0.42
1:C:672:THR:HG23	1:C:675:ARG:HH11	1.83	0.42
1:A:190:ARG:HD3	1:A:218:TYR:CE1	2.53	0.42
1:A:57:ALA:HA	1:A:60:ASN:ND2	2.35	0.42
1:A:91:THR:HG21	1:B:56:PHE:CD2	2.54	0.42
1:C:607:PHE:O	1:C:611:ILE:HG12	2.19	0.42
1:D:24:GLN:NE2	1:D:279:LYS:H	2.17	0.42
1:D:398:THR:HA	1:D:443:THR:O	2.20	0.42
1:D:105:GLY:O	1:D:107:HIS:ND1	2.53	0.42
1:D:201:VAL:O	1:D:205:VAL:HG23	2.19	0.42
1:D:323:TRP:CZ3	1:D:325:GLN:HB2	2.54	0.42
1:A:41:PHE:CE2	1:A:297:ARG:HD2	2.54	0.42
1:B:105:GLY:O	1:B:107:HIS:ND1	2.50	0.42
1:C:314:ASP:OD1	1:C:315:CYS:N	2.53	0.42
1:C:407:MET:N	1:C:422:GLU:O	2.50	0.42
1:C:76:PHE:CD1	1:C:99:PRO:HD2	2.54	0.42
1:D:451:GLY:HA3	1:D:464:VAL:HG23	2.02	0.42
1:D:15:GLY:N	1:D:72:ALA:O	2.44	0.42
1:A:153:ALA:HA	1:A:158:TRP:HB2	2.02	0.42
1:A:522:ALA:H	1:A:525:ILE:HD12	1.85	0.42
1:B:363:LEU:HA	1:B:368:PRO:HA	2.02	0.42
1:C:702:TYR:CE2	1:C:704:LEU:HD23	2.55	0.42
1:D:451:GLY:HA2	1:D:461:ASN:O	2.19	0.42
1:D:462:GLY:O	1:D:466:GLU:HG3	2.19	0.42
1:A:369:ARG:NH1	1:A:385:ASP:OD1	2.45	0.42
1:A:418:ASN:HD21	1:A:441:LYS:HA	1.85	0.42
1:B:505:LYS:NZ	1:B:697:LYS:HA	2.35	0.42
1:C:409:LYS:HD2	1:C:422:GLU:CD	2.40	0.42
1:C:480:THR:H	2:C:1101:ZK1:CAT	2.32	0.42
1:D:211:ILE:HD12	1:D:213:LYS:HD2	2.02	0.42
1:A:317:ALA:O	1:A:320:ALA:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLY:HA2	1:A:383:THR:OG1	2.20	0.41
1:B:190:ARG:HD3	1:B:218:TYR:HE1	1.83	0.41
1:C:232:LEU:HD23	1:C:363:LEU:HD13	2.00	0.41
1:C:387:THR:C	1:C:389:GLY:H	2.23	0.41
1:C:595:SER:HB2	1:D:578:TRP:CG	2.55	0.41
1:D:595:SER:CA	1:D:599:ARG:HB3	2.42	0.41
1:A:521:LEU:HD21	1:A:525:ILE:HB	2.01	0.41
1:A:809:VAL:HA	1:A:812:ILE:HG12	2.01	0.41
1:B:11:SER:OG	1:B:44:THR:OG1	2.26	0.41
1:C:395:VAL:H	1:C:440:TYR:HA	1.85	0.41
1:D:101:PHE:HA	1:D:102:PRO:HD3	1.91	0.41
1:D:309:ARG:HG2	1:D:311:ASN:N	2.30	0.41
1:D:348:ASP:OD2	1:D:350:ASN:HB2	2.20	0.41
1:D:445:VAL:HG23	1:D:466:GLU:OE2	2.19	0.41
1:C:91:THR:HG21	1:D:56:PHE:CD2	2.55	0.41
1:C:91:THR:HG21	1:D:56:PHE:CE2	2.55	0.41
1:D:742:LEU:O	1:D:746:VAL:HG23	2.21	0.41
1:A:130:TRP:CE2	1:A:191:ARG:HD3	2.55	0.41
1:A:506:LYS:HA	1:A:507:PRO:HD3	1.68	0.41
1:B:16:GLY:H	1:B:65:GLN:NE2	2.11	0.41
1:B:540:LEU:HB2	1:B:576:SER:OG	2.19	0.41
1:D:651:ASP:HA	1:D:682:PHE:CD1	2.55	0.41
1:A:107:HIS:HA	1:A:108:PRO:HD3	1.82	0.41
1:A:143:LEU:HD21	1:B:147:GLN:NE2	2.33	0.41
1:C:597:SER:O	1:C:600:ILE:HG12	2.19	0.41
1:C:744:THR:O	1:C:748:LEU:HG	2.20	0.41
1:C:814:PHE:HA	1:C:817:LYS:HD2	2.02	0.41
1:D:505:LYS:NZ	1:D:697:LYS:HA	2.35	0.41
1:B:595:SER:H	1:B:599:ARG:HG3	1.86	0.41
1:C:101:PHE:HA	1:C:102:PRO:HD3	1.77	0.41
1:C:651:ASP:HA	1:C:682:PHE:HB3	2.01	0.41
1:D:394:THR:HA	1:D:439:LYS:HB2	2.03	0.41
1:B:13:GLN:HB3	1:B:70:VAL:HG12	2.02	0.41
1:B:99:PRO:O	1:B:114:ARG:HB2	2.20	0.41
1:A:113:MET:O	1:A:115:PRO:HD3	2.20	0.41
1:A:763:LYS:O	1:A:767:TRP:HB2	2.21	0.41
1:A:91:THR:HG21	1:B:56:PHE:CE2	2.55	0.41
1:C:93:HIS:ND1	1:C:322:PRO:HG2	2.35	0.41
1:C:460:TRP:CE3	1:C:464:VAL:HG11	2.56	0.41
1:C:651:ASP:HA	1:C:682:PHE:CD1	2.56	0.41
1:D:54:ASN:OD1	1:D:56:PHE:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:708:MET:O	1:D:712:ILE:HG12	2.20	0.41
1:A:590:ASP:O	1:A:591:ILE:HG22	2.20	0.41
1:B:742:LEU:O	1:B:746:VAL:HG23	2.20	0.41
1:C:466:GLU:O	1:C:472:ALA:N	2.50	0.41
1:C:608:PHE:HZ	1:D:796:PHE:HE1	1.69	0.41
1:C:651:ASP:OD2	1:C:684:ARG:HA	2.21	0.41
1:D:255:VAL:O	1:D:259:ILE:HG12	2.20	0.41
1:D:42:ARG:HG2	1:D:43:LEU:O	2.21	0.41
1:D:493:LYS:HA	1:D:494:PRO:HD3	1.91	0.41
1:A:175:GLU:HA	1:A:178:ARG:HH11	1.85	0.41
1:A:480:THR:H	2:A:1101:ZK1:CAT	2.34	0.41
1:A:811:LEU:HA	1:A:814:PHE:HD2	1.86	0.41
1:C:17:LEU:HB2	1:C:75:GLY:HA3	2.02	0.41
1:C:374:TRP:CH2	1:C:376:GLU:HA	2.56	0.41
1:A:101:PHE:HA	1:A:102:PRO:HD3	1.76	0.41
1:B:207:GLN:O	1:B:211:ILE:HG12	2.21	0.41
1:A:56:PHE:CE2	1:B:91:THR:HG21	2.56	0.41
1:D:112:GLN:HE21	1:D:352:LYS:HA	1.85	0.41
1:A:576:SER:HA	1:A:579:PHE:HB3	2.02	0.41
1:A:595:SER:HA	1:A:599:ARG:HH11	1.86	0.41
1:B:513:GLY:O	1:B:515:PHE:N	2.49	0.41
1:C:115:PRO:HB3	1:C:356:TYR:CG	2.56	0.41
1:C:651:ASP:OD1	1:C:652:SER:N	2.54	0.41
1:A:204:ILE:O	1:A:208:VAL:HG23	2.20	0.40
1:A:384:GLU:O	1:A:386:ASP:N	2.54	0.40
1:A:595:SER:H	1:A:599:ARG:NE	2.19	0.40
1:B:79:LYS:O	1:B:82:VAL:HG12	2.20	0.40
1:C:96:PHE:CE2	1:C:98:THR:HB	2.56	0.40
1:D:232:LEU:HD23	1:D:363:LEU:HD22	2.03	0.40
1:A:293:THR:O	1:A:297:ARG:HG2	2.21	0.40
1:D:141:ARG:HH22	1:D:196:CYS:N	2.18	0.40
1:D:475:ALA:HB3	1:D:735:ALA:HB3	2.03	0.40
1:B:453:ARG:HD2	1:B:460:TRP:CE2	2.57	0.40
1:B:664:ILE:HB	1:B:667:PHE:HD2	1.86	0.40
1:D:135:TYR:O	1:D:162:ALA:HA	2.22	0.40
1:D:505:LYS:HA	1:D:720:THR:HG22	2.03	0.40
1:B:25:GLU:OE1	1:B:25:GLU:N	2.48	0.40
1:B:41:PHE:HZ	1:B:297:ARG:HG3	1.86	0.40
1:B:394:THR:O	1:B:440:TYR:HA	2.22	0.40
1:C:150:LEU:HD23	1:C:160:VAL:HG21	2.03	0.40
1:C:590:ASP:C	1:C:592:SER:H	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:GLU:N	1:D:25:GLU:OE1	2.47	0.40
1:A:348:ASP:HB3	1:A:354:ILE:HG21	2.03	0.40
1:C:121:LEU:HA	1:C:245:PHE:HZ	1.87	0.40
1:C:526:TRP:O	1:C:530:VAL:HG23	2.22	0.40
1:C:57:ALA:HA	1:C:60:ASN:ND2	2.36	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 PDB entries followed by that with respect to all EM entries.

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	779/1057 (74%)	729 (94%)	35 (4%)	15 (2%)	9	47
1	B	776/1057 (73%)	728 (94%)	37 (5%)	11 (1%)	13	54
1	C	779/1057 (74%)	726 (93%)	38 (5%)	15 (2%)	9	47
1	D	776/1057 (73%)	728 (94%)	35 (4%)	13 (2%)	11	50
All	All	3110/4228 (74%)	2911 (94%)	145 (5%)	54 (2%)	15	50

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ASP
1	A	591	ILE
1	B	395	VAL
1	B	512	PRO
1	C	591	ILE
1	D	395	VAL
1	D	590	ASP
1	D	591	ILE
1	A	587	GLN
1	B	587	GLN

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Mol	Chain	Res	Type
1	B	590	ASP
1	B	595	SER
1	B	785	SER
1	C	173	LYS
1	C	174	ASP
1	C	587	GLN
1	D	587	GLN
1	D	595	SER
1	D	596	LEU
1	A	174	ASP
1	A	394	THR
1	A	575	ASN
1	A	594	ARG
1	A	595	SER
1	A	596	LEU
1	B	173	LYS
1	B	174	ASP
1	B	437	GLY
1	C	437	GLY
1	C	590	ASP
1	C	594	ARG
1	C	595	SER
1	C	596	LEU
1	C	787	LEU
1	D	520	PRO
1	D	594	ARG
1	A	173	LYS
1	A	389	GLY
1	A	437	GLY
1	C	390	LEU
1	C	394	THR
1	A	765	LYS
1	B	591	ILE
1	C	765	LYS
1	D	514	VAL
1	A	787	LEU
1	B	478	PRO
1	C	574	PHE
1	D	174	ASP
1	D	512	PRO
1	D	782	GLU
1	A	478	PRO

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Mol	Chain	Res	Type
1	C	16	GLY
1	D	437	GLY

### 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 PDB entries followed by that with respect to all EM entries.

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	666/888 (75%)	666 (100%)	0	100	100
1	B	664/888 (75%)	664 (100%)	0	100	100
1	C	666/888 (75%)	666 (100%)	0	100	100
1	D	664/888 (75%)	664 (100%)	0	100	100
All	All	2660/3552 (75%)	2660 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	35	GLN
1	A	65	GLN
1	A	147	GLN
1	A	214	HIS
1	A	246	GLN
1	A	311	ASN
1	A	355	ASN
1	A	587	GLN
1	A	619	ASN
1	A	642	GLN
1	A	756	GLN
1	B	24	GLN
1	B	46	HIS
1	B	65	GLN
1	B	83	ASN

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Mol	Chain	Res	Type
1	B	147	GLN
1	B	214	HIS
1	B	325	GLN
1	B	337	GLN
1	B	355	ASN
1	B	412	HIS
1	B	587	GLN
1	B	619	ASN
1	B	642	GLN
1	C	24	GLN
1	C	65	GLN
1	C	83	ASN
1	C	112	GLN
1	C	147	GLN
1	C	311	ASN
1	C	325	GLN
1	C	337	GLN
1	C	344	ASN
1	C	355	ASN
1	C	587	GLN
1	C	619	ASN
1	C	642	GLN
1	C	756	GLN
1	D	24	GLN
1	D	65	GLN
1	D	147	GLN
1	D	344	ASN
1	D	412	HIS
1	D	435	HIS
1	D	587	GLN
1	D	619	ASN
1	D	642	GLN
1	D	714	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ZK1	A	1101	-	28,29,29	3.11	10 (35%)	36,45,45	1.66	7 (19%)
3	NAG	A	1102	-	14,14,15	0.26	0	15,19,21	0.40	0
2	ZK1	B	1101	-	28,29,29	3.15	10 (35%)	36,45,45	1.60	6 (16%)
3	NAG	B	1102	-	14,14,15	0.20	0	15,19,21	0.49	0
2	ZK1	C	1101	-	28,29,29	3.11	11 (39%)	36,45,45	1.64	7 (19%)
3	NAG	C	1102	-	14,14,15	0.20	0	15,19,21	0.49	0
2	ZK1	D	1101	-	28,29,29	3.15	11 (39%)	36,45,45	1.61	7 (19%)
3	NAG	D	1102	-	14,14,15	0.18	0	15,19,21	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZK1	A	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	A	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	B	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	B	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	C	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	C	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	D	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	D	1102	-	-	0/6/23/26	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ZK1	PBA-OAD	-3.71	1.46	1.54
2	B	1101	ZK1	PBA-OAD	-3.68	1.46	1.54
2	C	1101	ZK1	PBA-OAD	-3.67	1.46	1.54
2	D	1101	ZK1	PBA-OAD	-3.65	1.46	1.54
2	C	1101	ZK1	CAU-NAY	-2.09	1.35	1.38
2	A	1101	ZK1	CAU-NAY	-2.07	1.35	1.38
2	C	1101	ZK1	CAV-NAP	2.06	1.38	1.35
2	D	1101	ZK1	CAR-NAX	2.07	1.45	1.41
2	D	1101	ZK1	CAV-NAP	2.09	1.38	1.35
2	B	1101	ZK1	CAV-NAP	2.13	1.38	1.35
2	C	1101	ZK1	CAI-CAR	2.32	1.41	1.37
2	A	1101	ZK1	CAI-CAR	2.39	1.41	1.37
2	D	1101	ZK1	CAI-CAR	2.39	1.41	1.37
2	B	1101	ZK1	CAI-CAR	2.45	1.42	1.37
2	C	1101	ZK1	CAW-NAY	4.03	1.45	1.40
2	A	1101	ZK1	CAW-NAY	4.10	1.45	1.40
2	B	1101	ZK1	CAW-NAY	4.19	1.46	1.40
2	C	1101	ZK1	CAJ-CAS	4.30	1.44	1.37
2	D	1101	ZK1	CAW-NAY	4.35	1.46	1.40
2	B	1101	ZK1	PBA-OAE	4.38	1.65	1.54
2	C	1101	ZK1	PBA-OAE	4.39	1.65	1.54
2	A	1101	ZK1	CAJ-CAS	4.42	1.44	1.37
2	A	1101	ZK1	PBA-OAE	4.43	1.65	1.54
2	D	1101	ZK1	CAJ-CAS	4.44	1.44	1.37
2	D	1101	ZK1	PBA-OAE	4.44	1.65	1.54
2	B	1101	ZK1	CAJ-CAS	4.50	1.44	1.37
2	A	1101	ZK1	CAT-NAP	5.80	1.43	1.33
2	C	1101	ZK1	CAT-NAP	5.86	1.43	1.33
2	D	1101	ZK1	CAT-NAP	6.00	1.43	1.33
2	B	1101	ZK1	CAT-NAP	6.09	1.44	1.33
2	B	1101	ZK1	OAB-CAU	6.42	1.40	1.24
2	A	1101	ZK1	OAB-CAU	6.45	1.40	1.24
2	C	1101	ZK1	OAB-CAU	6.47	1.40	1.24
2	A	1101	ZK1	OAA-CAT	6.48	1.40	1.24
2	D	1101	ZK1	OAB-CAU	6.49	1.40	1.24
2	D	1101	ZK1	OAA-CAT	6.56	1.41	1.24
2	B	1101	ZK1	OAA-CAT	6.59	1.41	1.24
2	C	1101	ZK1	OAA-CAT	6.60	1.41	1.24
2	A	1101	ZK1	PBA-OAC	6.86	1.65	1.50
2	C	1101	ZK1	PBA-OAC	6.89	1.65	1.50
2	B	1101	ZK1	PBA-OAC	6.89	1.65	1.50
2	D	1101	ZK1	PBA-OAC	6.93	1.65	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	ZK1	CAI-CAR-NAX	-3.32	118.15	122.69
2	B	1101	ZK1	CAI-CAR-NAX	-3.16	118.37	122.69
2	A	1101	ZK1	CAI-CAR-NAX	-3.03	118.55	122.69
2	C	1101	ZK1	CAI-CAR-NAX	-2.92	118.69	122.69
2	A	1101	ZK1	FAG-CAZ-CAS	-2.43	108.33	112.69
2	B	1101	ZK1	FAG-CAZ-CAS	-2.42	108.34	112.69
2	C	1101	ZK1	FAG-CAZ-CAS	-2.41	108.35	112.69
2	D	1101	ZK1	FAG-CAZ-CAS	-2.34	108.47	112.69
2	C	1101	ZK1	CAM-NAX-CAR	2.03	121.02	116.33
2	D	1101	ZK1	CAM-NAX-CAR	2.07	121.11	116.33
2	A	1101	ZK1	CAM-NAX-CAR	2.09	121.16	116.33
2	B	1101	ZK1	CAO-NAY-CAU	2.18	120.43	117.79
2	D	1101	ZK1	CAO-NAY-CAU	2.26	120.53	117.79
2	C	1101	ZK1	CAO-NAY-CAU	2.73	121.09	117.79
2	A	1101	ZK1	CAO-NAY-CAU	2.76	121.12	117.79
2	A	1101	ZK1	CAV-CAW-NAY	3.47	120.23	117.66
2	C	1101	ZK1	CAV-CAW-NAY	3.49	120.25	117.66
2	B	1101	ZK1	CAV-CAW-NAY	3.61	120.34	117.66
2	B	1101	ZK1	CAN-NAX-CAM	3.67	119.35	111.57
2	D	1101	ZK1	CAN-NAX-CAM	3.69	119.39	111.57
2	D	1101	ZK1	CAV-CAW-NAY	3.69	120.40	117.66
2	C	1101	ZK1	CAN-NAX-CAM	3.81	119.65	111.57
2	D	1101	ZK1	CAT-NAP-CAV	3.85	119.43	116.42
2	A	1101	ZK1	CAN-NAX-CAM	3.87	119.76	111.57
2	B	1101	ZK1	CAT-NAP-CAV	4.04	119.58	116.42
2	C	1101	ZK1	CAT-NAP-CAV	4.21	119.71	116.42
2	A	1101	ZK1	CAT-NAP-CAV	4.25	119.74	116.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ZK1	4	0
3	A	1102	NAG	2	0
2	B	1101	ZK1	2	0
2	C	1101	ZK1	3	0
3	C	1102	NAG	2	0
2	D	1101	ZK1	2	0
3	D	1102	NAG	3	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.