



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:09 am GMT

PDB ID : 2NSU
EMDB ID: : EMD-1288
Title : Crystal structure of the ectodomain of human transferrin receptor fitted into a cryo-EM reconstruction of canine parvovirus and feline transferrin receptor complex
Authors : Hafenstein, S.; Kostyuchenko, V.A.; Rossmann, M.G.
Deposited on : 2006-11-06
Resolution : 27.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
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) : recalc29047

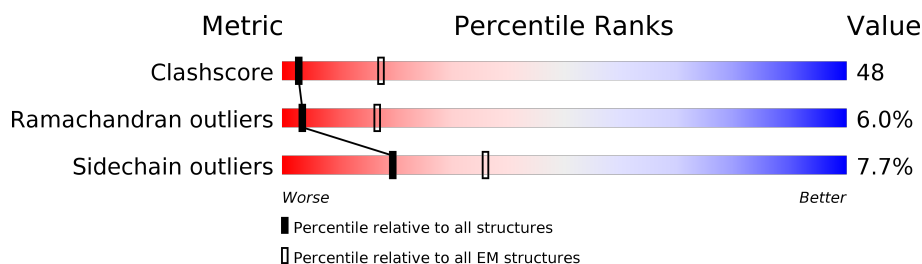
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 27.00 Å.

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



Metric	Whole archive (#Entries)	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 ≥ 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	639	 40% 49% 9% .
1	B	639	 41% 49% 10% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10112 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 Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	639	Total	C	N	O	S	0	0
			5056	3244	846	952	14		
1	B	639	Total	C	N	O	S	0	0
			5056	3244	846	952	14		

There are 6 discrepancies between the modelled and reference sequences:

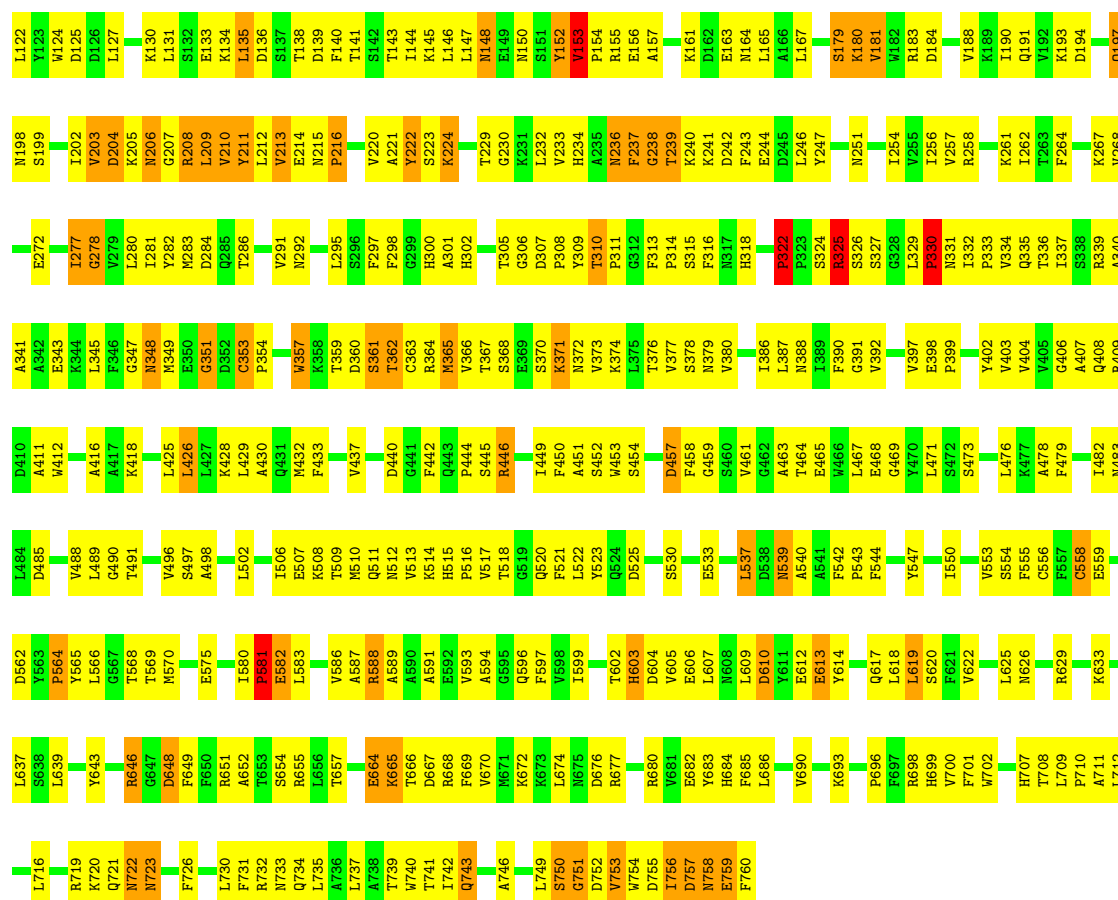
Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	GLY	VARIANT	UNP P02786
A	172	GLU	GLN	SEE REMARK 999	UNP P02786
A	613	GLU	ARG	SEE REMARK 999	UNP P02786
B	142	SER	GLY	VARIANT	UNP P02786
B	172	GLU	GLN	SEE REMARK 999	UNP P02786
B	613	GLU	ARG	SEE REMARK 999	UNP P02786

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

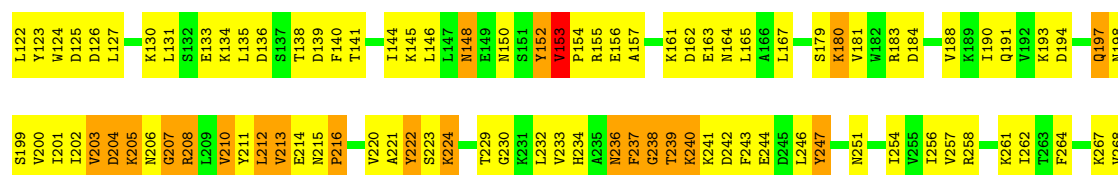
• Molecule 1: Transferrin receptor protein 1

Chain A: 



• Molecule 1: Transferrin receptor protein 1

Chain B: 



P710	K633	C558	N483	B410	R339	E272
A711	L637	E559	L484	A411	A340	A341
L712	S638	D562	D485	W412	A342	I277
L716	L639	Y563	V488	G415	E343	G278
R719	Y643	P564	L489	A416	K344	V279
K720	R646	Y565	G490	A417	L345	L280
Q721	G647	L566	T491	K418	F346	I281
N722	D648	G567	V496	L425	G347	Y282
N723	F649	T568	S497	L426	N348	M283
F726	F650	T569	A498	L427	E350	G285
L730	R651	M570	S499	K428	G351	T286
F731	A652	D571	F500	L429	D352	K287
R732	S654	E575	L501	A430	C353	F289
N733	R655	I580	L502	Q431	P354	
Q734	L656	P581	I506	N432	W357	V291
L735	T657	E582	F507	F433	K358	N292
W740	F660	L583	K508	V437	T359	L295
I741	E664	R584	M509	D440	D360	S296
I742	K665	V585	M510	G441	S361	F297
Q743	T666	V586	Q511	T362	T362	F298
A746	D667	A587	N512	F442	C363	G299
L749	R668	R588	V513	Q443	R364	H300
S750	D669	A589	K514	P444	M365	A301
G751	F669	A590	H515	R445	V366	H302
D752	V670	E592	P517	I449	T367	T305
V753	K671	V593	T518	F450	E368	G306
W754	K672	G595	Q519	A451	S370	D307
D755	L674	Q596	F520	S452	K371	P308
I756	N675	F597	L522	W453	N372	Y309
D757	D676	V598	Y523	S454	V373	T310
N758	R677	I599	Q524	D457	K374	P311
E759	R680	T602	D525	F458	L375	G312
F760	V681	R603	S530	G459	T376	F313
	E682	D604	E533	S460	V377	P314
	Y683	V605	L537	V461	S378	S315
	H684	E606	D538	G462	N379	F316
	F685	L607	A540	A463	V380	H317
	L686	W608	N539	T464	I366	H318
	V690	D610	A541	E465	L387	P322
	S691	E613	F542	L467	N388	P323
	P692	Y614	G469	G466	V392	S324
	K693	Q617	F544	Y470	V397	S326
	R698	L618	Y547	L471	E398	S327
	H699	L619	I550	S472	P399	G328
	V700	S620	L476	A478		L329
	F701	N626	K477	F479	Y402	P330
	W702	R629	A478	I482	N331	N331
	H707		S553		V403	T332
	T708		S554		P333	V334
	L709		F555		V405	V334
			F556		G406	Q335
			C556		A407	T336
			F557		Q408	T337
					R409	S338

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction of each particle	Depositor
Microscope	FEI/PHILIPS CM200 FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.96	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	54000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.38	0/5177	0.61	1/7021 (0.0%)
1	B	0.38	0/5177	0.61	1/7021 (0.0%)
All	All	0.38	0/10354	0.61	2/14042 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	751	GLY	N-CA-C	-5.19	100.12	113.10
1	A	751	GLY	N-CA-C	-5.14	100.25	113.10

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	5056	0	4982	506	0
1	B	5056	0	4982	481	0
All	All	10112	0	9964	970	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 48.

All (970) 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:153:VAL:HG13	1:A:154:PRO:HD3	1.20	1.17
1:B:153:VAL:HG13	1:B:154:PRO:HD3	1.21	1.09
1:B:210:VAL:HG13	1:B:211:TYR:H	1.22	1.05
1:B:359:THR:HG22	1:B:360:ASP:H	1.22	1.04
1:A:359:THR:HG22	1:A:360:ASP:H	1.25	0.99
1:B:348:ASN:HB3	1:B:371:LYS:HE3	1.47	0.96
1:A:203:VAL:HB	1:A:208:ARG:HA	1.49	0.94
1:B:306:GLY:HA2	1:B:461:VAL:HA	1.50	0.94
1:B:184:ASP:HB3	1:B:388:ASN:HB2	1.46	0.94
1:A:348:ASN:HB3	1:A:371:LYS:HE3	1.49	0.93
1:B:708:THR:HG22	1:B:711:ALA:H	1.31	0.93
1:A:209:LEU:HG	1:A:210:VAL:H	1.35	0.92
1:A:354:PRO:HD3	1:A:365:MET:SD	2.09	0.92
1:A:130:LYS:HE3	1:A:134:LYS:HD3	1.51	0.90
1:A:349:MET:HB2	1:A:364:ARG:HG3	1.54	0.90
1:A:140:PHE:HE1	1:A:588:ARG:HA	1.36	0.90
1:B:130:LYS:HE3	1:B:134:LYS:HD3	1.54	0.89
1:B:349:MET:HB2	1:B:364:ARG:HG3	1.54	0.89
1:A:161:LYS:HA	1:A:164:ASN:HD22	1.37	0.89
1:A:184:ASP:HB3	1:A:388:ASN:HB2	1.52	0.89
1:B:444:PRO:HB3	1:B:602:THR:HG21	1.56	0.88
1:A:153:VAL:HG13	1:A:154:PRO:CD	2.04	0.88
1:B:161:LYS:HA	1:B:164:ASN:HD22	1.39	0.88
1:B:300:HIS:HE1	1:B:302:HIS:HB3	1.39	0.88
1:A:239:THR:HB	1:A:244:GLU:HG2	1.55	0.88
1:B:354:PRO:HD3	1:B:365:MET:SD	2.14	0.87
1:B:153:VAL:CG1	1:B:154:PRO:HD3	2.05	0.87
1:A:353:CYS:HA	1:A:365:MET:SD	2.15	0.86
1:B:140:PHE:HE1	1:B:588:ARG:HA	1.38	0.86
1:B:667:ASP:HB3	1:B:670:VAL:HG22	1.57	0.86
1:A:708:THR:HG22	1:A:711:ALA:H	1.39	0.85
1:B:239:THR:HB	1:B:244:GLU:HG2	1.57	0.85
1:A:153:VAL:CG1	1:A:154:PRO:HD3	2.03	0.85
1:B:426:LEU:HD21	1:B:450:PHE:HB3	1.58	0.85
1:B:353:CYS:HA	1:B:365:MET:SD	2.16	0.84
1:B:708:THR:HG23	1:B:710:PRO:HD2	1.59	0.84
1:A:667:ASP:HB3	1:A:670:VAL:HG22	1.57	0.84
1:B:201:ILE:HD11	1:B:208:ARG:HB2	1.57	0.84
1:A:426:LEU:HD21	1:A:450:PHE:HB3	1.59	0.83
1:A:306:GLY:HA2	1:A:461:VAL:HA	1.59	0.83
1:A:442:PHE:CZ	1:A:444:PRO:HG3	2.13	0.83
1:A:708:THR:HG23	1:A:710:PRO:HD2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:ARG:HH11	1:B:646:ARG:HG2	1.42	0.83
1:A:758:ASN:HB2	1:B:183:ARG:O	1.79	0.83
1:B:442:PHE:CZ	1:B:444:PRO:HG3	2.14	0.83
1:B:310:THR:OG1	1:B:468:GLU:OE1	1.96	0.82
1:A:465:GLU:OE2	1:A:468:GLU:CD	2.17	0.82
1:B:300:HIS:CE1	1:B:302:HIS:HB3	2.14	0.82
1:B:153:VAL:HG13	1:B:154:PRO:CD	2.06	0.82
1:A:300:HIS:CE1	1:A:302:HIS:HB3	2.14	0.81
1:B:280:LEU:HD12	1:B:337:ILE:HD13	1.61	0.81
1:A:300:HIS:HE1	1:A:302:HIS:HB3	1.42	0.81
1:B:465:GLU:OE2	1:B:468:GLU:CD	2.19	0.80
1:A:140:PHE:CE1	1:A:588:ARG:HA	2.17	0.80
1:A:310:THR:OG1	1:A:468:GLU:OE1	1.98	0.80
1:A:444:PRO:HB3	1:A:602:THR:HG21	1.64	0.80
1:B:150:ASN:HA	1:B:153:VAL:HG12	1.64	0.79
1:A:646:ARG:HG2	1:A:646:ARG:HH11	1.46	0.79
1:B:199:SER:HB2	1:B:212:LEU:HD11	1.63	0.79
1:B:310:THR:HG21	1:B:315:SER:HB3	1.63	0.79
1:A:465:GLU:OE2	1:A:468:GLU:OE2	2.01	0.79
1:B:210:VAL:HG13	1:B:211:TYR:N	1.97	0.79
1:B:685:PHE:O	1:B:700:VAL:HG22	1.84	0.78
1:B:465:GLU:OE2	1:B:468:GLU:OE1	2.01	0.78
1:A:208:ARG:HD2	1:A:208:ARG:O	1.83	0.78
1:B:309:TYR:HE2	1:B:325:ARG:HA	1.47	0.78
1:B:140:PHE:CE1	1:B:588:ARG:HA	2.18	0.78
1:A:310:THR:HG21	1:A:315:SER:HB3	1.66	0.77
1:B:496:VAL:HG11	1:B:506:ILE:HG21	1.65	0.77
1:A:496:VAL:HG11	1:A:506:ILE:HG21	1.65	0.77
1:A:188:VAL:CG2	1:A:386:ILE:HD11	2.14	0.76
1:A:280:LEU:HD12	1:A:337:ILE:HD13	1.65	0.76
1:B:238:GLY:HA3	1:B:267:LYS:HG2	1.67	0.76
1:B:191:GLN:HE22	1:B:223:SER:H	1.33	0.76
1:B:232:LEU:HD22	1:B:373:VAL:HG11	1.68	0.75
1:A:150:ASN:HA	1:A:153:VAL:HG12	1.68	0.75
1:A:310:THR:O	1:A:468:GLU:OE1	2.04	0.75
1:B:518:THR:HG22	1:B:520:GLN:H	1.50	0.75
1:A:309:TYR:HE2	1:A:325:ARG:HA	1.50	0.75
1:A:465:GLU:CD	1:A:468:GLU:OE2	2.25	0.75
1:A:220:VAL:HG21	1:A:334:VAL:HG12	1.69	0.75
1:A:278:GLY:H	1:A:332:ILE:HG23	1.53	0.74
1:B:278:GLY:H	1:B:332:ILE:HG23	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:HIS:O	1:B:322:PRO:HB3	1.88	0.73
1:A:188:VAL:HG21	1:A:386:ILE:HD11	1.70	0.73
1:A:183:ARG:O	1:B:758:ASN:HB2	1.87	0.73
1:A:191:GLN:HE22	1:A:223:SER:H	1.34	0.73
1:A:232:LEU:HD22	1:A:373:VAL:HG11	1.70	0.73
1:A:397:VAL:C	1:A:399:PRO:HD3	2.09	0.72
1:A:229:THR:HB	1:A:374:LYS:HG3	1.71	0.72
1:B:398:GLU:HB2	1:B:446:ARG:HG2	1.72	0.72
1:B:295:LEU:HD21	1:B:568:THR:HG21	1.70	0.72
1:A:310:THR:O	1:A:310:THR:OG1	2.00	0.72
1:B:183:ARG:NH1	1:B:387:LEU:HD21	2.04	0.72
1:B:310:THR:OG1	1:B:310:THR:O	2.03	0.72
1:A:740:TRP:CZ2	1:B:314:PRO:HB2	2.25	0.72
1:A:518:THR:HG22	1:A:520:GLN:H	1.54	0.72
1:B:407:ALA:HB3	1:B:426:LEU:HD12	1.70	0.72
1:B:305:THR:HG23	1:B:464:THR:HG21	1.71	0.72
1:A:685:PHE:O	1:A:700:VAL:HG22	1.90	0.71
1:A:407:ALA:HB3	1:A:426:LEU:HD12	1.72	0.71
1:B:465:GLU:CD	1:B:468:GLU:OE2	2.29	0.71
1:A:295:LEU:HD21	1:A:568:THR:HG21	1.70	0.71
1:B:359:THR:HG22	1:B:360:ASP:N	2.03	0.71
1:A:515:HIS:HD2	1:A:517:VAL:H	1.37	0.71
1:B:229:THR:HB	1:B:374:LYS:CG	2.21	0.71
1:B:188:VAL:CG2	1:B:386:ILE:HD11	2.21	0.70
1:A:212:LEU:HD21	1:A:215:ASN:HD21	1.55	0.70
1:B:229:THR:HB	1:B:374:LYS:HG3	1.70	0.70
1:B:341:ALA:O	1:B:345:LEU:HD23	1.91	0.70
1:A:318:HIS:O	1:A:322:PRO:HB3	1.90	0.70
1:A:130:LYS:HE2	1:A:440:ASP:OD1	1.92	0.70
1:A:229:THR:HB	1:A:374:LYS:CG	2.21	0.70
1:B:297:PHE:O	1:B:336:THR:HG21	1.90	0.70
1:B:238:GLY:HA3	1:B:267:LYS:CG	2.22	0.70
1:B:397:VAL:C	1:B:399:PRO:HD3	2.12	0.70
1:A:708:THR:CG2	1:A:710:PRO:HD2	2.21	0.70
1:B:625:LEU:HD21	1:B:639:LEU:HD11	1.73	0.70
1:B:732:ARG:HH11	1:B:732:ARG:HG3	1.55	0.70
1:A:239:THR:HB	1:A:244:GLU:CG	2.22	0.69
1:B:150:ASN:HA	1:B:153:VAL:CG1	2.22	0.69
1:A:626:ASN:HB3	1:A:629:ARG:HH21	1.58	0.69
1:B:204:ASP:C	1:B:206:ASN:H	1.95	0.69
1:A:183:ARG:NH1	1:A:387:LEU:HD21	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:ARG:HG3	1:A:732:ARG:HH11	1.58	0.69
1:A:349:MET:HG2	1:A:367:THR:HA	1.73	0.69
1:B:506:ILE:O	1:B:510:MET:HG3	1.93	0.69
1:A:214:GLU:O	1:A:216:PRO:HD3	1.94	0.68
1:B:330:PRO:O	1:B:331:ASN:HB3	1.94	0.68
1:B:515:HIS:HD2	1:B:517:VAL:H	1.38	0.68
1:B:213:VAL:HG11	1:B:345:LEU:HD21	1.74	0.68
1:B:307:ASP:HB3	1:B:465:GLU:OE1	1.94	0.68
1:A:398:GLU:HB2	1:A:446:ARG:HG2	1.75	0.68
1:B:239:THR:HB	1:B:244:GLU:CG	2.24	0.68
1:B:220:VAL:HG21	1:B:334:VAL:HG12	1.75	0.68
1:B:349:MET:HG2	1:B:367:THR:HA	1.76	0.68
1:B:351:GLY:O	1:B:364:ARG:HD3	1.93	0.68
1:B:208:ARG:HG2	1:B:208:ARG:O	1.93	0.68
1:A:297:PHE:O	1:A:336:THR:HG21	1.94	0.68
1:B:309:TYR:CE2	1:B:325:ARG:HA	2.28	0.68
1:B:254:ILE:HA	1:B:277:ILE:O	1.94	0.68
1:B:313:PHE:O	1:B:468:GLU:OE1	2.12	0.68
1:B:542:PHE:HB3	1:B:543:PRO:HD3	1.75	0.68
1:B:232:LEU:HB3	1:B:367:THR:HG23	1.76	0.67
1:B:310:THR:O	1:B:468:GLU:OE1	2.11	0.67
1:A:140:PHE:O	1:A:144:ILE:HG13	1.94	0.67
1:A:254:ILE:HA	1:A:277:ILE:O	1.95	0.67
1:B:167:LEU:HD22	1:B:183:ARG:HH22	1.58	0.67
1:B:337:ILE:HG23	1:B:341:ALA:HB3	1.77	0.67
1:A:490:GLY:HA3	1:A:559:GLU:HG2	1.76	0.67
1:A:359:THR:HG22	1:A:360:ASP:N	2.06	0.67
1:A:341:ALA:O	1:A:345:LEU:HD23	1.95	0.67
1:A:351:GLY:O	1:A:364:ARG:HD3	1.95	0.67
1:A:488:VAL:O	1:A:489:LEU:HD12	1.94	0.67
1:B:300:HIS:HE2	1:B:459:GLY:CA	2.07	0.67
1:A:330:PRO:O	1:A:331:ASN:HB3	1.93	0.66
1:B:188:VAL:HG21	1:B:386:ILE:HD11	1.76	0.66
1:B:465:GLU:OE2	1:B:468:GLU:OE2	2.11	0.66
1:A:309:TYR:CE2	1:A:325:ARG:HA	2.30	0.66
1:A:337:ILE:HG23	1:A:341:ALA:HB3	1.76	0.66
1:B:183:ARG:HH12	1:B:387:LEU:HD21	1.58	0.66
1:A:150:ASN:HA	1:A:153:VAL:CG1	2.26	0.66
1:A:311:PRO:O	1:A:693:LYS:HA	1.96	0.65
1:A:664:GLU:H	1:A:664:GLU:CD	2.00	0.65
1:A:209:LEU:CG	1:A:210:VAL:H	2.07	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:LEU:HD23	1:B:699:HIS:CA	2.26	0.65
1:A:246:LEU:HD12	1:A:247:TYR:N	2.12	0.65
1:B:140:PHE:O	1:B:144:ILE:HG13	1.96	0.65
1:A:155:ARG:HH21	1:A:165:LEU:HD22	1.60	0.65
1:A:686:LEU:HD23	1:A:699:HIS:CA	2.25	0.65
1:B:353:CYS:HB2	1:B:363:CYS:O	1.96	0.65
1:B:626:ASN:HB3	1:B:629:ARG:HH21	1.62	0.65
1:B:359:THR:CG2	1:B:360:ASP:H	2.02	0.65
1:B:349:MET:HB2	1:B:364:ARG:CG	2.27	0.65
1:A:238:GLY:HA3	1:A:267:LYS:HG2	1.80	0.64
1:A:353:CYS:HB2	1:A:363:CYS:O	1.97	0.64
1:B:664:GLU:H	1:B:664:GLU:CD	2.01	0.64
1:B:139:ASP:OD1	1:B:141:THR:HG22	1.97	0.64
1:B:229:THR:HB	1:B:374:LYS:CB	2.28	0.64
1:A:232:LEU:HD11	1:A:256:ILE:HG13	1.80	0.64
1:A:625:LEU:HD21	1:A:639:LEU:HD11	1.79	0.64
1:A:686:LEU:HD23	1:A:699:HIS:HA	1.79	0.64
1:A:758:ASN:HD22	1:A:758:ASN:N	1.96	0.64
1:B:238:GLY:O	1:B:240:LYS:N	2.31	0.64
1:B:191:GLN:NE2	1:B:223:SER:H	1.96	0.64
1:B:349:MET:HB3	1:B:366:VAL:O	1.98	0.64
1:A:542:PHE:HB3	1:A:543:PRO:HD3	1.80	0.64
1:A:654:SER:O	1:A:657:THR:HG22	1.98	0.64
1:B:716:LEU:HD13	1:B:731:PHE:CE1	2.33	0.64
1:A:238:GLY:O	1:A:240:LYS:N	2.29	0.63
1:A:488:VAL:C	1:A:489:LEU:HD12	2.18	0.63
1:B:220:VAL:CG1	1:B:301:ALA:HB2	2.28	0.63
1:A:183:ARG:HH12	1:A:387:LEU:HD21	1.61	0.63
1:B:625:LEU:CD2	1:B:639:LEU:HD11	2.28	0.63
1:B:155:ARG:HH21	1:B:165:LEU:HD22	1.64	0.63
1:A:232:LEU:HB3	1:A:367:THR:HG23	1.78	0.63
1:B:200:VAL:HG23	1:B:213:VAL:HB	1.79	0.63
1:B:646:ARG:HG2	1:B:646:ARG:NH1	2.11	0.63
1:B:156:GLU:HG2	1:B:157:ALA:H	1.64	0.63
1:A:240:LYS:C	1:A:242:ASP:H	2.00	0.63
1:A:130:LYS:HE2	1:A:440:ASP:CG	2.19	0.63
1:B:130:LYS:HE2	1:B:440:ASP:OD1	1.97	0.63
1:A:232:LEU:HD21	1:A:256:ILE:HD11	1.79	0.63
1:A:349:MET:HB3	1:A:366:VAL:O	1.99	0.63
1:A:349:MET:HB2	1:A:364:ARG:CG	2.27	0.63
1:B:446:ARG:HD2	1:B:479:PHE:CE2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD22	1:A:183:ARG:HH22	1.63	0.63
1:A:465:GLU:OE2	1:A:468:GLU:OE1	2.16	0.63
1:B:324:SER:HB3	1:B:325:ARG:HE	1.64	0.63
1:B:488:VAL:O	1:B:489:LEU:HD12	1.99	0.63
1:B:690:VAL:HG23	1:B:698:ARG:HG2	1.81	0.63
1:A:555:PHE:CE2	1:A:593:VAL:HG23	2.34	0.62
1:A:664:GLU:OE1	1:A:667:ASP:HB2	1.98	0.62
1:B:152:TYR:HA	1:B:161:LYS:HE2	1.82	0.62
1:A:539:ASN:HD22	1:A:540:ALA:N	1.97	0.62
1:A:515:HIS:CD2	1:A:517:VAL:H	2.16	0.62
1:B:348:ASN:HD22	1:B:348:ASN:N	1.97	0.62
1:A:204:ASP:C	1:A:206:ASN:H	2.02	0.62
1:A:229:THR:HB	1:A:374:LYS:CB	2.30	0.62
1:B:201:ILE:HD13	1:B:212:LEU:HA	1.80	0.62
1:B:191:GLN:HE22	1:B:223:SER:N	1.98	0.62
1:A:278:GLY:H	1:A:332:ILE:CG2	2.12	0.62
1:A:506:ILE:O	1:A:510:MET:HG3	2.00	0.62
1:A:210:VAL:HG22	1:A:211:TYR:H	1.63	0.62
1:A:313:PHE:O	1:A:468:GLU:OE1	2.18	0.62
1:B:167:LEU:CD2	1:B:183:ARG:HH22	2.11	0.62
1:A:191:GLN:HE22	1:A:223:SER:N	1.98	0.62
1:B:708:THR:CG2	1:B:710:PRO:HD2	2.27	0.62
1:A:191:GLN:NE2	1:A:223:SER:H	1.97	0.62
1:A:446:ARG:HD2	1:A:479:PHE:CE2	2.34	0.62
1:B:664:GLU:OE1	1:B:667:ASP:HB2	1.99	0.62
1:A:156:GLU:HG2	1:A:157:ALA:H	1.64	0.61
1:B:278:GLY:HA2	1:B:333:PRO:O	2.00	0.61
1:A:238:GLY:HA3	1:A:267:LYS:CG	2.29	0.61
1:A:349:MET:HA	1:A:367:THR:HA	1.83	0.61
1:B:240:LYS:C	1:B:242:ASP:H	2.04	0.61
1:B:194:ASP:HB3	1:B:378:SER:O	2.00	0.61
1:B:238:GLY:C	1:B:240:LYS:H	2.02	0.61
1:B:246:LEU:HD12	1:B:247:TYR:N	2.16	0.61
1:B:490:GLY:HA3	1:B:559:GLU:HG2	1.82	0.61
1:A:446:ARG:H	1:A:602:THR:CG2	2.13	0.61
1:B:236:ASN:OD1	1:B:258:ARG:HD3	2.00	0.61
1:A:238:GLY:H	1:A:257:VAL:HB	1.65	0.61
1:B:686:LEU:HD23	1:B:699:HIS:HA	1.82	0.61
1:A:236:ASN:OD1	1:A:258:ARG:HD3	2.00	0.61
1:A:307:ASP:HB3	1:A:465:GLU:OE1	2.01	0.61
1:A:605:VAL:HG11	1:A:665:LYS:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HD12	1:B:337:ILE:CD1	2.30	0.61
1:B:758:ASN:N	1:B:758:ASN:HD22	1.96	0.61
1:A:220:VAL:CG1	1:A:301:ALA:HB2	2.31	0.60
1:B:349:MET:HA	1:B:367:THR:HA	1.84	0.60
1:B:368:SER:OG	1:B:371:LYS:HE2	2.01	0.60
1:B:295:LEU:HD11	1:B:568:THR:OG1	2.01	0.60
1:A:139:ASP:OD1	1:A:141:THR:HG22	2.01	0.60
1:A:167:LEU:CD2	1:A:183:ARG:HH22	2.15	0.60
1:A:655:ARG:NH1	1:A:751:GLY:HA2	2.16	0.60
1:B:515:HIS:CD2	1:B:517:VAL:H	2.18	0.60
1:B:131:LEU:O	1:B:135:LEU:HD23	2.00	0.60
1:B:188:VAL:HG21	1:B:461:VAL:HG11	1.82	0.60
1:A:336:THR:O	1:A:337:ILE:HD12	2.01	0.60
1:B:654:SER:O	1:B:657:THR:HG22	2.01	0.60
1:A:152:TYR:HA	1:A:161:LYS:HE2	1.84	0.60
1:A:210:VAL:HG13	1:A:211:TYR:O	2.01	0.60
1:A:690:VAL:HG23	1:A:698:ARG:HG2	1.82	0.60
1:B:256:ILE:HD11	1:B:349:MET:HE1	1.82	0.60
1:A:220:VAL:HG12	1:A:301:ALA:HB2	1.82	0.59
1:B:488:VAL:C	1:B:489:LEU:HD12	2.23	0.59
1:B:130:LYS:O	1:B:134:LYS:HG2	2.02	0.59
1:B:310:THR:OG1	1:B:465:GLU:OE2	2.20	0.59
1:A:131:LEU:O	1:A:135:LEU:HD23	2.02	0.59
1:A:348:ASN:HD22	1:A:348:ASN:N	2.00	0.59
1:A:368:SER:OG	1:A:371:LYS:HE2	2.01	0.59
1:A:209:LEU:HG	1:A:210:VAL:N	2.11	0.59
1:A:324:SER:HB3	1:A:325:ARG:HE	1.68	0.59
1:A:314:PRO:HB2	1:B:740:TRP:CZ2	2.37	0.59
1:A:298:PHE:HB2	1:A:412:TRP:CD2	2.38	0.59
1:B:167:LEU:HD22	1:B:183:ARG:NH2	2.17	0.59
1:B:324:SER:CB	1:B:325:ARG:HE	2.15	0.59
1:A:237:PHE:CD2	1:A:258:ARG:HB2	2.38	0.59
1:A:345:LEU:O	1:A:349:MET:HG3	2.03	0.59
1:B:214:GLU:O	1:B:216:PRO:HD3	2.03	0.59
1:A:238:GLY:C	1:A:240:LYS:H	2.04	0.59
1:A:307:ASP:H	1:A:461:VAL:HG13	1.68	0.59
1:B:130:LYS:HE2	1:B:440:ASP:CG	2.23	0.59
1:A:719:ARG:HH11	1:A:719:ARG:HG3	1.68	0.59
1:B:588:ARG:HH11	1:B:588:ARG:HG3	1.67	0.59
1:A:515:HIS:CD2	1:A:516:PRO:HD2	2.38	0.58
1:B:664:GLU:C	1:B:666:THR:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:VAL:HG22	1:B:479:PHE:CZ	2.37	0.58
1:B:220:VAL:HG12	1:B:301:ALA:HB2	1.85	0.58
1:B:237:PHE:HB2	1:B:243:PHE:HE1	1.67	0.58
1:B:268:VAL:HG21	1:B:334:VAL:HG21	1.86	0.58
1:A:300:HIS:O	1:A:301:ALA:HB3	2.02	0.58
1:B:655:ARG:NH1	1:B:751:GLY:HA2	2.18	0.58
1:A:280:LEU:HD12	1:A:337:ILE:CD1	2.33	0.58
1:B:756:ILE:HG22	1:B:756:ILE:O	2.04	0.58
1:A:625:LEU:CD2	1:A:639:LEU:HD11	2.33	0.58
1:A:202:ILE:HB	1:A:210:VAL:HG11	1.86	0.58
1:B:238:GLY:O	1:B:262:ILE:HD11	2.04	0.58
1:B:278:GLY:H	1:B:332:ILE:CG2	2.16	0.58
1:A:264:PHE:CE2	1:A:281:ILE:HG21	2.39	0.57
1:A:446:ARG:H	1:A:602:THR:HG23	1.68	0.57
1:A:238:GLY:O	1:A:262:ILE:HD11	2.04	0.57
1:A:699:HIS:HD2	1:A:702:TRP:H	1.51	0.57
1:B:442:PHE:CE2	1:B:444:PRO:HG3	2.38	0.57
1:B:555:PHE:CE2	1:B:593:VAL:HG23	2.39	0.57
1:A:664:GLU:C	1:A:666:THR:H	2.08	0.57
1:A:749:LEU:O	1:A:750:SER:CB	2.53	0.57
1:B:719:ARG:HD3	1:B:726:PHE:CD2	2.40	0.57
1:A:433:PHE:O	1:A:437:VAL:HG23	2.04	0.57
1:A:672:LYS:HD3	1:A:676:ASP:OD2	2.05	0.57
1:A:670:VAL:O	1:A:674:LEU:HG	2.05	0.57
1:A:758:ASN:HD22	1:A:758:ASN:H	1.50	0.57
1:B:239:THR:C	1:B:241:LYS:H	2.08	0.57
1:A:453:TRP:CD2	1:A:463:ALA:HB2	2.40	0.57
1:B:272:GLU:OE2	1:B:330:PRO:O	2.23	0.57
1:B:426:LEU:CD2	1:B:450:PHE:HB3	2.31	0.57
1:A:496:VAL:HG11	1:A:506:ILE:CG2	2.35	0.57
1:A:403:VAL:HG22	1:A:479:PHE:CZ	2.40	0.57
1:A:298:PHE:HE2	1:A:457:ASP:HB3	1.70	0.57
1:B:336:THR:O	1:B:337:ILE:HD12	2.05	0.56
1:B:496:VAL:HG11	1:B:506:ILE:CG2	2.34	0.56
1:A:194:ASP:HB3	1:A:378:SER:O	2.05	0.56
1:B:758:ASN:H	1:B:758:ASN:HD22	1.52	0.56
1:A:256:ILE:HD11	1:A:349:MET:HE1	1.87	0.56
1:B:237:PHE:CD2	1:B:258:ARG:HB2	2.40	0.56
1:A:167:LEU:HD22	1:A:183:ARG:NH2	2.20	0.56
1:A:272:GLU:OE2	1:A:330:PRO:O	2.23	0.56
1:B:680:ARG:HB3	1:B:684:HIS:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PHE:HB2	1:A:243:PHE:HE1	1.69	0.56
1:A:339:ARG:O	1:A:343:GLU:HG2	2.05	0.56
1:A:398:GLU:N	1:A:399:PRO:HD3	2.21	0.56
1:B:345:LEU:O	1:B:349:MET:HG3	2.04	0.56
1:A:238:GLY:N	1:A:257:VAL:HB	2.20	0.56
1:A:453:TRP:CG	1:A:463:ALA:HB2	2.41	0.56
1:A:719:ARG:HD3	1:A:726:PHE:CD2	2.41	0.56
1:B:300:HIS:O	1:B:301:ALA:HB3	2.06	0.56
1:B:286:THR:CG2	1:B:360:ASP:HB2	2.35	0.56
1:B:719:ARG:HH11	1:B:719:ARG:HG3	1.70	0.56
1:A:442:PHE:CE2	1:A:444:PRO:HG3	2.40	0.56
1:A:300:HIS:HE2	1:A:459:GLY:CA	2.18	0.56
1:B:232:LEU:HB3	1:B:367:THR:CG2	2.35	0.56
1:B:618:LEU:HD11	1:B:742:ILE:HD13	1.87	0.56
1:B:756:ILE:H	1:B:756:ILE:HD12	1.71	0.56
1:A:539:ASN:O	1:A:542:PHE:N	2.38	0.56
1:A:680:ARG:HB3	1:A:684:HIS:HD2	1.71	0.56
1:A:286:THR:CG2	1:A:360:ASP:HB2	2.36	0.55
1:B:539:ASN:HD22	1:B:540:ALA:N	2.04	0.55
1:B:676:ASP:O	1:B:680:ARG:HG3	2.06	0.55
1:B:759:GLU:HG3	1:B:760:PHE:N	2.21	0.55
1:A:654:SER:HA	1:A:657:THR:HG22	1.89	0.55
1:A:756:ILE:HG22	1:A:756:ILE:O	2.05	0.55
1:B:565:TYR:CE1	1:B:575:GLU:HB3	2.41	0.55
1:A:426:LEU:CD2	1:A:450:PHE:HB3	2.34	0.55
1:A:565:TYR:CE1	1:A:575:GLU:HB3	2.42	0.55
1:A:607:LEU:CD1	1:A:609:LEU:HG	2.37	0.55
1:B:446:ARG:H	1:B:602:THR:HG23	1.70	0.55
1:B:752:ASP:O	1:B:753:VAL:HB	2.06	0.55
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.88	0.55
1:A:156:GLU:HG2	1:A:157:ALA:N	2.22	0.55
1:B:398:GLU:N	1:B:399:PRO:HD3	2.22	0.55
1:A:237:PHE:CD1	1:A:261:LYS:HG3	2.42	0.55
1:A:619:LEU:HD23	1:A:620:SER:N	2.22	0.55
1:B:699:HIS:HD2	1:B:702:TRP:H	1.55	0.55
1:A:306:GLY:HA2	1:A:461:VAL:CA	2.34	0.55
1:A:471:LEU:HD13	1:A:547:TYR:OH	2.07	0.55
1:A:324:SER:CB	1:A:325:ARG:HE	2.19	0.54
1:B:618:LEU:HD13	1:B:701:PHE:HZ	1.72	0.54
1:A:232:LEU:HB3	1:A:367:THR:CG2	2.36	0.54
1:A:425:LEU:HD22	1:A:591:ALA:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLN:HE21	1:B:215:ASN:HB3	1.71	0.54
1:B:446:ARG:H	1:B:602:THR:CG2	2.20	0.54
1:B:222:TYR:HB3	1:B:329:LEU:HD23	1.89	0.54
1:A:335:GLN:NE2	1:A:336:THR:HG22	2.23	0.54
1:A:155:ARG:HA	1:A:161:LYS:HB2	1.90	0.54
1:A:268:VAL:HG21	1:A:334:VAL:HG21	1.87	0.54
1:A:347:GLY:C	1:A:348:ASN:HD22	2.11	0.54
1:B:190:ILE:HG13	1:B:458:PHE:CD2	2.43	0.54
1:B:238:GLY:H	1:B:257:VAL:HB	1.72	0.54
1:B:502:LEU:O	1:B:506:ILE:HG13	2.08	0.54
1:B:135:LEU:HD22	1:B:432:MET:SD	2.47	0.54
1:A:278:GLY:HA2	1:A:333:PRO:O	2.07	0.54
1:A:488:VAL:HG13	1:A:586:VAL:HG11	1.90	0.54
1:A:758:ASN:CB	1:B:183:ARG:O	2.55	0.54
1:B:232:LEU:HD11	1:B:256:ILE:HG13	1.90	0.54
1:A:654:SER:C	1:A:657:THR:HG22	2.28	0.54
1:B:237:PHE:CD1	1:B:261:LYS:HG3	2.43	0.54
1:B:471:LEU:HD13	1:B:547:TYR:OH	2.08	0.54
1:B:515:HIS:CD2	1:B:516:PRO:HD2	2.43	0.54
1:B:672:LYS:HD3	1:B:676:ASP:OD2	2.08	0.54
1:A:212:LEU:HD21	1:A:215:ASN:ND2	2.23	0.53
1:A:540:ALA:O	1:A:543:PRO:HD2	2.08	0.53
1:A:588:ARG:HG3	1:A:588:ARG:HH11	1.73	0.53
1:B:311:PRO:O	1:B:693:LYS:HA	2.08	0.53
1:B:749:LEU:O	1:B:750:SER:CB	2.55	0.53
1:A:131:LEU:HD22	1:A:599:ILE:HD11	1.89	0.53
1:A:513:VAL:HG21	1:A:593:VAL:HG12	1.89	0.53
1:B:756:ILE:N	1:B:756:ILE:HD12	2.23	0.53
1:A:667:ASP:OD1	1:A:669:PHE:HB3	2.09	0.53
1:B:156:GLU:HG2	1:B:157:ALA:N	2.22	0.53
1:B:201:ILE:HB	1:B:212:LEU:HD12	1.90	0.53
1:B:654:SER:HA	1:B:657:THR:HG22	1.89	0.53
1:A:496:VAL:CG1	1:A:506:ILE:HD13	2.39	0.53
1:A:646:ARG:NH1	1:A:646:ARG:HG2	2.17	0.53
1:A:743:GLN:O	1:A:746:ALA:HB3	2.08	0.53
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.91	0.53
1:A:239:THR:C	1:A:241:LYS:H	2.11	0.53
1:A:232:LEU:CD2	1:A:256:ILE:HD11	2.38	0.53
1:B:240:LYS:HA	1:B:262:ILE:HD13	1.90	0.53
1:A:236:ASN:HB2	1:A:357:TRP:CD1	2.44	0.53
1:B:236:ASN:HB2	1:B:357:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:ARG:CG	1:B:719:ARG:HH11	2.22	0.53
1:A:197:GLN:HE21	1:A:215:ASN:HB3	1.74	0.52
1:A:295:LEU:HD11	1:A:568:THR:OG1	2.08	0.52
1:A:719:ARG:HH11	1:A:719:ARG:CG	2.22	0.52
1:A:145:LYS:O	1:A:148:ASN:HB2	2.09	0.52
1:A:256:ILE:CD1	1:A:349:MET:HE1	2.38	0.52
1:A:361:SER:O	1:A:362:THR:CB	2.58	0.52
1:A:135:LEU:HD22	1:A:432:MET:SD	2.49	0.52
1:B:199:SER:CB	1:B:212:LEU:HD11	2.38	0.52
1:B:212:LEU:O	1:B:213:VAL:C	2.47	0.52
1:B:540:ALA:O	1:B:543:PRO:HD2	2.10	0.52
1:B:619:LEU:HD23	1:B:620:SER:N	2.23	0.52
1:A:515:HIS:CD2	1:A:516:PRO:CD	2.92	0.52
1:B:206:ASN:O	1:B:207:GLY:O	2.26	0.52
1:B:347:GLY:C	1:B:348:ASN:HD22	2.11	0.52
1:B:580:ILE:HG23	1:B:580:ILE:O	2.08	0.52
1:B:698:ARG:HA	1:B:707:HIS:NE2	2.24	0.52
1:A:473:SER:O	1:A:476:LEU:HB2	2.09	0.52
1:B:201:ILE:HD12	1:B:202:ILE:N	2.25	0.52
1:B:298:PHE:HE2	1:B:457:ASP:HB3	1.74	0.52
1:B:523:TYR:HE1	1:B:530:SER:OG	1.91	0.52
1:A:648:ASP:OD2	1:A:757:ASP:OD2	2.28	0.52
1:A:752:ASP:O	1:A:753:VAL:HB	2.09	0.52
1:B:201:ILE:HD13	1:B:212:LEU:CA	2.40	0.52
1:A:212:LEU:CD2	1:A:215:ASN:HD21	2.21	0.52
1:A:618:LEU:HD11	1:A:742:ILE:HD13	1.92	0.52
1:B:339:ARG:O	1:B:343:GLU:HG2	2.09	0.52
1:B:433:PHE:O	1:B:437:VAL:HG23	2.09	0.52
1:B:498:ALA:HB2	1:B:553:VAL:HA	1.91	0.52
1:A:668:ARG:HD2	1:B:669:PHE:CD2	2.45	0.52
1:A:124:TRP:HH2	1:A:596:GLN:HG2	1.75	0.52
1:A:163:GLU:O	1:A:167:LEU:HG	2.10	0.52
1:A:188:VAL:HG21	1:A:461:VAL:HG11	1.92	0.52
1:B:409:ARG:NH2	1:B:454:SER:HB2	2.24	0.52
1:B:553:VAL:HG22	1:B:554:SER:N	2.25	0.52
1:B:564:PRO:HG2	1:B:565:TYR:H	1.74	0.52
1:A:453:TRP:CE3	1:A:463:ALA:HA	2.44	0.52
1:B:146:LEU:HD23	1:B:146:LEU:O	2.10	0.52
1:B:335:GLN:NE2	1:B:336:THR:HG22	2.25	0.52
1:A:188:VAL:HG22	1:A:386:ILE:HD11	1.90	0.51
1:B:513:VAL:HG21	1:B:593:VAL:HG12	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ASP:O	1:A:680:ARG:HG3	2.10	0.51
1:B:232:LEU:HD21	1:B:256:ILE:HD11	1.91	0.51
1:B:198:ASN:OD1	1:B:378:SER:N	2.43	0.51
1:A:502:LEU:O	1:A:506:ILE:HG13	2.10	0.51
1:B:453:TRP:CG	1:B:463:ALA:HB2	2.45	0.51
1:B:607:LEU:CD1	1:B:609:LEU:HG	2.40	0.51
1:B:238:GLY:HA3	1:B:267:LYS:CD	2.41	0.51
1:B:238:GLY:N	1:B:257:VAL:HB	2.26	0.51
1:B:282:TYR:HE1	1:B:284:ASP:HB3	1.76	0.51
1:B:286:THR:HG21	1:B:360:ASP:HB2	1.93	0.51
1:A:210:VAL:HG22	1:A:211:TYR:N	2.25	0.51
1:A:498:ALA:HB2	1:A:553:VAL:HA	1.92	0.51
1:B:127:LEU:HD22	1:B:127:LEU:N	2.25	0.51
1:B:749:LEU:O	1:B:750:SER:HB3	2.11	0.51
1:A:232:LEU:HD11	1:A:256:ILE:CG1	2.40	0.51
1:A:349:MET:HA	1:A:368:SER:N	2.26	0.51
1:A:199:SER:O	1:A:376:THR:HG22	2.11	0.51
1:A:483:ASN:HD21	1:A:540:ALA:HB3	1.75	0.51
1:B:155:ARG:HA	1:B:161:LYS:HB2	1.91	0.51
1:B:750:SER:OG	1:B:751:GLY:N	2.42	0.51
1:A:130:LYS:O	1:A:134:LYS:HG2	2.10	0.51
1:A:300:HIS:HE2	1:A:459:GLY:N	2.09	0.51
1:B:256:ILE:CD1	1:B:349:MET:HE1	2.40	0.51
1:A:316:PHE:CZ	1:B:740:TRP:NE1	2.75	0.51
1:A:425:LEU:O	1:A:429:LEU:HB2	2.11	0.51
1:A:618:LEU:HD21	1:A:742:ILE:HG23	1.92	0.51
1:A:716:LEU:HD13	1:A:731:PHE:CE1	2.46	0.51
1:B:204:ASP:C	1:B:206:ASN:N	2.63	0.51
1:B:605:VAL:HG11	1:B:665:LYS:HB3	1.92	0.51
1:A:669:PHE:CD2	1:B:668:ARG:HD2	2.46	0.51
1:B:239:THR:C	1:B:241:LYS:N	2.64	0.51
1:B:199:SER:O	1:B:376:THR:HG22	2.11	0.51
1:A:700:VAL:HG23	1:A:701:PHE:CD1	2.46	0.51
1:B:145:LYS:O	1:B:148:ASN:HB2	2.11	0.51
1:B:361:SER:O	1:B:362:THR:CB	2.59	0.51
1:B:307:ASP:H	1:B:461:VAL:HG13	1.76	0.51
1:B:667:ASP:OD1	1:B:669:PHE:HB3	2.12	0.51
1:B:682:GLU:OE2	1:B:699:HIS:CE1	2.64	0.50
1:A:539:ASN:HD22	1:A:539:ASN:C	2.15	0.50
1:A:537:LEU:HD22	1:A:542:PHE:CE2	2.46	0.50
1:A:759:GLU:O	1:A:760:PHE:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ASN:O	1:B:542:PHE:N	2.39	0.50
1:B:655:ARG:HH11	1:B:751:GLY:HA2	1.77	0.50
1:A:446:ARG:HH12	1:A:602:THR:HA	1.76	0.50
1:A:677:ARG:NE	1:A:750:SER:HB2	2.26	0.50
1:B:278:GLY:HA2	1:B:333:PRO:HG2	1.93	0.50
1:A:224:LYS:HA	1:A:224:LYS:HE3	1.94	0.50
1:A:553:VAL:HG22	1:A:554:SER:N	2.27	0.50
1:B:349:MET:HA	1:B:368:SER:N	2.26	0.50
1:B:568:THR:HG23	1:B:570:MET:H	1.76	0.50
1:A:240:LYS:HG2	1:A:240:LYS:O	2.12	0.50
1:B:291:VAL:HG13	1:B:292:ASN:N	2.27	0.50
1:B:453:TRP:CD2	1:B:463:ALA:HB2	2.47	0.50
1:B:648:ASP:OD2	1:B:757:ASP:OD2	2.29	0.50
1:A:238:GLY:HA3	1:A:267:LYS:HD3	1.94	0.50
1:A:392:VAL:HG12	1:A:449:ILE:HB	1.94	0.50
1:A:307:ASP:N	1:A:461:VAL:HG13	2.26	0.50
1:B:197:GLN:NE2	1:B:215:ASN:HB3	2.27	0.50
1:B:565:TYR:HE1	1:B:575:GLU:HB3	1.75	0.50
1:B:654:SER:C	1:B:657:THR:HG22	2.32	0.50
1:A:222:TYR:HB3	1:A:329:LEU:HD23	1.93	0.50
1:A:282:TYR:HE1	1:A:284:ASP:HB3	1.77	0.50
1:A:238:GLY:HA3	1:A:267:LYS:CD	2.42	0.50
1:A:483:ASN:ND2	1:A:540:ALA:HB3	2.27	0.50
1:A:667:ASP:HB3	1:A:670:VAL:CG2	2.36	0.50
1:A:655:ARG:HH11	1:A:751:GLY:HA2	1.76	0.50
1:B:224:LYS:HA	1:B:224:LYS:HE3	1.93	0.50
1:A:239:THR:HB	1:A:244:GLU:CD	2.33	0.49
1:A:305:THR:HG23	1:A:464:THR:HG21	1.93	0.49
1:A:553:VAL:HG21	1:A:597:PHE:CE2	2.46	0.49
1:B:300:HIS:HE2	1:B:459:GLY:N	2.10	0.49
1:B:667:ASP:HB3	1:B:670:VAL:CG2	2.37	0.49
1:A:239:THR:C	1:A:241:LYS:N	2.65	0.49
1:A:278:GLY:HA2	1:A:333:PRO:HG2	1.94	0.49
1:A:409:ARG:HB2	1:A:452:SER:OG	2.11	0.49
1:A:408:GLN:HB3	1:A:485:ASP:OD1	2.12	0.49
1:A:618:LEU:HD13	1:A:701:PHE:HZ	1.76	0.49
1:A:759:GLU:HG3	1:A:760:PHE:N	2.27	0.49
1:A:496:VAL:HG11	1:A:506:ILE:HD13	1.94	0.49
1:A:238:GLY:HA2	1:A:257:VAL:HG11	1.95	0.49
1:A:286:THR:HG21	1:A:360:ASP:HB2	1.94	0.49
1:A:682:GLU:OE2	1:A:699:HIS:CE1	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:VAL:CG1	1:B:506:ILE:HD13	2.42	0.49
1:B:618:LEU:HD21	1:B:742:ILE:HG23	1.94	0.49
1:B:670:VAL:O	1:B:674:LEU:HG	2.12	0.49
1:A:180:LYS:N	1:A:180:LYS:HD2	2.28	0.49
1:A:213:VAL:O	1:A:214:GLU:HB2	2.13	0.49
1:A:523:TYR:HE1	1:A:530:SER:OG	1.95	0.49
1:B:210:VAL:CG1	1:B:211:TYR:N	2.69	0.49
1:B:411:ALA:HA	1:B:457:ASP:OD2	2.13	0.49
1:A:197:GLN:NE2	1:A:215:ASN:HB3	2.28	0.49
1:A:240:LYS:HA	1:A:262:ILE:HD13	1.95	0.49
1:A:756:ILE:N	1:A:756:ILE:HD12	2.27	0.49
1:B:497:SER:OG	1:B:533:GLU:HB3	2.12	0.49
1:A:568:THR:HG23	1:A:570:MET:H	1.77	0.49
1:A:756:ILE:H	1:A:756:ILE:HD12	1.77	0.49
1:B:146:LEU:HD23	1:B:146:LEU:C	2.32	0.49
1:A:209:LEU:O	1:A:210:VAL:HG12	2.13	0.49
1:A:297:PHE:N	1:A:297:PHE:CD1	2.81	0.49
1:A:580:ILE:O	1:A:580:ILE:HG23	2.13	0.49
1:B:237:PHE:HB2	1:B:243:PHE:CE1	2.46	0.49
1:B:361:SER:O	1:B:362:THR:HB	2.13	0.49
1:A:467:LEU:HD21	1:A:544:PHE:CZ	2.48	0.49
1:A:361:SER:O	1:A:362:THR:HB	2.12	0.48
1:B:264:PHE:CE2	1:B:281:ILE:HG21	2.47	0.48
1:A:237:PHE:HB2	1:A:243:PHE:CE1	2.47	0.48
1:B:163:GLU:O	1:B:167:LEU:HG	2.12	0.48
1:B:240:LYS:O	1:B:241:LYS:HB3	2.13	0.48
1:B:325:ARG:HG2	1:B:326:SER:N	2.28	0.48
1:B:680:ARG:HB3	1:B:684:HIS:CD2	2.47	0.48
1:A:240:LYS:O	1:A:241:LYS:HB3	2.13	0.48
1:B:712:LEU:C	1:B:712:LEU:HD23	2.34	0.48
1:B:677:ARG:NE	1:B:750:SER:HB2	2.27	0.48
1:A:133:GLU:HA	1:A:136:ASP:HB2	1.96	0.48
1:A:203:VAL:HG23	1:A:206:ASN:O	2.14	0.48
1:A:749:LEU:O	1:A:750:SER:HB3	2.14	0.48
1:B:232:LEU:HD13	1:B:254:ILE:HG22	1.96	0.48
1:B:359:THR:CG2	1:B:360:ASP:N	2.72	0.48
1:A:131:LEU:HD22	1:A:599:ILE:CD1	2.43	0.48
1:A:680:ARG:HB3	1:A:684:HIS:CD2	2.48	0.48
1:A:699:HIS:CD2	1:A:701:PHE:HB2	2.49	0.48
1:A:700:VAL:HG23	1:A:701:PHE:HD1	1.79	0.48
1:B:386:ILE:CG2	1:B:454:SER:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:GLN:HB3	1:B:485:ASP:OD1	2.14	0.48
1:A:153:VAL:HG22	1:A:154:PRO:CD	2.43	0.48
1:A:232:LEU:HB2	1:A:373:VAL:CG1	2.44	0.48
1:A:305:THR:O	1:A:305:THR:HG23	2.13	0.48
1:A:198:ASN:OD1	1:A:378:SER:N	2.44	0.48
1:A:430:ALA:HA	1:A:450:PHE:CZ	2.49	0.48
1:B:305:THR:O	1:B:305:THR:HG23	2.13	0.48
1:B:753:VAL:HG12	1:B:754:TRP:CG	2.48	0.48
1:A:237:PHE:HD2	1:A:258:ARG:HB2	1.78	0.48
1:A:677:ARG:HE	1:A:750:SER:HB2	1.78	0.48
1:A:712:LEU:HD23	1:A:712:LEU:C	2.33	0.48
1:B:152:TYR:HA	1:B:161:LYS:HB3	1.95	0.48
1:B:211:TYR:CG	1:B:212:LEU:N	2.81	0.48
1:B:297:PHE:N	1:B:297:PHE:CD1	2.82	0.48
1:A:236:ASN:O	1:A:243:PHE:HD1	1.97	0.48
1:B:343:GLU:OE2	1:B:362:THR:HG21	2.14	0.48
1:B:453:TRP:CE3	1:B:463:ALA:HA	2.49	0.48
1:B:537:LEU:HD22	1:B:542:PHE:CE2	2.48	0.48
1:B:425:LEU:HD22	1:B:591:ALA:HB2	1.96	0.48
1:A:386:ILE:CG2	1:A:454:SER:HB3	2.44	0.48
1:A:565:TYR:HE1	1:A:575:GLU:HB3	1.78	0.48
1:B:306:GLY:HA2	1:B:461:VAL:CA	2.32	0.48
1:B:230:GLY:O	1:B:372:ASN:HB2	2.13	0.48
1:B:515:HIS:CD2	1:B:516:PRO:CD	2.97	0.48
1:B:161:LYS:O	1:B:164:ASN:HB2	2.14	0.47
1:B:425:LEU:O	1:B:429:LEU:HB2	2.12	0.47
1:A:161:LYS:O	1:A:164:ASN:HB2	2.14	0.47
1:B:244:GLU:HA	1:B:244:GLU:OE1	2.14	0.47
1:A:180:LYS:H	1:A:180:LYS:HD2	1.80	0.47
1:A:357:TRP:O	1:A:359:THR:N	2.43	0.47
1:B:239:THR:HB	1:B:244:GLU:CD	2.34	0.47
1:B:409:ARG:HG2	1:B:409:ARG:HH11	1.79	0.47
1:B:698:ARG:HA	1:B:707:HIS:HE2	1.78	0.47
1:B:759:GLU:O	1:B:760:PHE:C	2.52	0.47
1:A:213:VAL:HG11	1:A:345:LEU:CD2	2.44	0.47
1:B:430:ALA:HA	1:B:450:PHE:CZ	2.50	0.47
1:B:651:ARG:HG2	1:B:651:ARG:HH11	1.79	0.47
1:A:152:TYR:HA	1:A:161:LYS:HB3	1.96	0.47
1:A:478:ALA:O	1:A:550:ILE:HD12	2.14	0.47
1:B:222:TYR:CE2	1:B:308:PRO:HG3	2.50	0.47
1:B:239:THR:O	1:B:243:PHE:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:O	1:A:243:PHE:HB2	2.15	0.47
1:A:409:ARG:HG2	1:A:409:ARG:HH11	1.78	0.47
1:B:180:LYS:HD2	1:B:180:LYS:N	2.30	0.47
1:A:465:GLU:HA	1:A:468:GLU:HB2	1.95	0.47
1:B:236:ASN:O	1:B:243:PHE:HD1	1.96	0.47
1:B:754:TRP:O	1:B:755:ASP:C	2.53	0.47
1:A:280:LEU:C	1:A:281:ILE:HD12	2.35	0.47
1:A:324:SER:O	1:A:325:ARG:HB3	2.14	0.47
1:A:497:SER:OG	1:A:533:GLU:HB3	2.14	0.47
1:B:203:VAL:HB	1:B:208:ARG:HA	1.97	0.47
1:B:330:PRO:O	1:B:331:ASN:CB	2.62	0.47
1:B:153:VAL:HG22	1:B:154:PRO:CD	2.45	0.47
1:B:759:GLU:HG3	1:B:760:PHE:H	1.80	0.47
1:A:359:THR:CG2	1:A:360:ASP:N	2.74	0.47
1:A:683:TYR:CD1	1:A:686:LEU:HD12	2.50	0.47
1:A:183:ARG:O	1:B:758:ASN:CB	2.58	0.47
1:A:244:GLU:OE1	1:A:244:GLU:HA	2.15	0.47
1:A:553:VAL:HG21	1:A:597:PHE:HE2	1.79	0.47
1:A:446:ARG:NH1	1:A:602:THR:HA	2.30	0.47
1:B:188:VAL:HG22	1:B:386:ILE:HD11	1.97	0.47
1:B:473:SER:O	1:B:476:LEU:HB2	2.15	0.47
1:A:353:CYS:HA	1:A:354:PRO:HD3	1.75	0.46
1:A:564:PRO:HG2	1:A:565:TYR:H	1.80	0.46
1:B:239:THR:O	1:B:241:LYS:N	2.48	0.46
1:B:639:LEU:HD23	1:B:643:TYR:HE1	1.80	0.46
1:A:134:LYS:O	1:A:138:THR:HG23	2.14	0.46
1:A:188:VAL:HG23	1:A:190:ILE:HD13	1.98	0.46
1:A:491:THR:HB	1:A:517:VAL:HG21	1.98	0.46
1:B:240:LYS:HG2	1:B:240:LYS:O	2.15	0.46
1:B:553:VAL:HG21	1:B:597:PHE:CE2	2.51	0.46
1:B:743:GLN:O	1:B:746:ALA:HB3	2.15	0.46
1:A:325:ARG:HG2	1:A:326:SER:N	2.29	0.46
1:A:580:ILE:N	1:A:581:PRO:HD3	2.31	0.46
1:A:730:LEU:HG	1:A:734:GLN:OE1	2.15	0.46
1:B:229:THR:HB	1:B:374:LYS:HB2	1.96	0.46
1:B:357:TRP:HE1	1:B:365:MET:CE	2.28	0.46
1:B:194:ASP:HB2	1:B:380:VAL:HG13	1.96	0.46
1:A:281:ILE:N	1:A:281:ILE:HD12	2.30	0.46
1:A:582:GLU:CD	1:A:582:GLU:H	2.18	0.46
1:A:654:SER:CA	1:A:657:THR:HG22	2.45	0.46
1:B:238:GLY:HA3	1:B:267:LYS:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:VAL:HG11	1:B:402:TYR:CE1	2.50	0.46
1:B:446:ARG:HH12	1:B:602:THR:HA	1.80	0.46
1:A:146:LEU:HD23	1:A:146:LEU:C	2.36	0.46
1:A:190:ILE:HG13	1:A:458:PHE:CD2	2.50	0.46
1:B:307:ASP:N	1:B:461:VAL:HG13	2.30	0.46
1:B:580:ILE:N	1:B:581:PRO:HD3	2.30	0.46
1:B:700:VAL:HG23	1:B:701:PHE:CD1	2.51	0.46
1:B:198:ASN:OD1	1:B:377:VAL:HA	2.16	0.46
1:A:190:ILE:CG2	1:A:191:GLN:N	2.78	0.46
1:A:232:LEU:CD1	1:A:256:ILE:HG13	2.45	0.46
1:A:409:ARG:NH2	1:A:454:SER:HB2	2.31	0.46
1:A:618:LEU:O	1:A:622:VAL:HG23	2.16	0.46
1:A:340:ALA:O	1:A:343:GLU:HB2	2.16	0.46
1:A:127:LEU:N	1:A:127:LEU:HD22	2.31	0.46
1:A:348:ASN:HB3	1:A:371:LYS:CE	2.35	0.46
1:A:508:LYS:O	1:A:512:ASN:ND2	2.49	0.46
1:A:698:ARG:HA	1:A:707:HIS:NE2	2.31	0.46
1:B:134:LYS:O	1:B:138:THR:HG23	2.16	0.46
1:A:553:VAL:HG11	1:A:597:PHE:CD2	2.51	0.45
1:A:664:GLU:CD	1:A:664:GLU:N	2.69	0.45
1:B:122:LEU:HD12	1:B:122:LEU:N	2.30	0.45
1:B:445:SER:N	1:B:602:THR:HG22	2.31	0.45
1:B:732:ARG:HG3	1:B:732:ARG:NH1	2.27	0.45
1:B:348:ASN:HB3	1:B:371:LYS:CE	2.33	0.45
1:A:555:PHE:HZ	1:A:594:ALA:HB2	1.81	0.45
1:A:731:PHE:O	1:A:732:ARG:C	2.54	0.45
1:A:750:SER:OG	1:A:751:GLY:N	2.48	0.45
1:A:607:LEU:HD11	1:A:609:LEU:HG	1.98	0.45
1:A:639:LEU:HD23	1:A:643:TYR:HE1	1.79	0.45
1:B:232:LEU:HB2	1:B:373:VAL:CG1	2.47	0.45
1:B:237:PHE:HD2	1:B:258:ARG:HB2	1.81	0.45
1:B:224:LYS:HB3	1:B:332:ILE:C	2.37	0.45
1:B:124:TRP:HH2	1:B:596:GLN:HG2	1.82	0.45
1:A:233:VAL:HG12	1:A:234:HIS:N	2.32	0.45
1:A:699:HIS:CD2	1:A:702:TRP:H	2.32	0.45
1:B:496:VAL:HG11	1:B:506:ILE:HD13	1.99	0.45
1:A:224:LYS:HB3	1:A:332:ILE:C	2.37	0.45
1:A:390:PHE:CD2	1:A:449:ILE:HD11	2.51	0.45
1:B:664:GLU:O	1:B:666:THR:N	2.50	0.45
1:A:291:VAL:HG13	1:A:292:ASN:N	2.31	0.45
1:A:754:TRP:O	1:A:755:ASP:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:TRP:O	1:B:359:THR:N	2.43	0.45
1:B:556:CYS:C	1:B:558:CYS:H	2.19	0.45
1:B:588:ARG:HG3	1:B:588:ARG:NH1	2.31	0.45
1:A:753:VAL:HG12	1:A:754:TRP:CG	2.51	0.45
1:B:428:LYS:HA	1:B:428:LYS:HD3	1.79	0.45
1:A:700:VAL:HG11	1:A:741:THR:HG21	1.97	0.45
1:A:721:GLN:O	1:A:723:ASN:N	2.50	0.45
1:B:211:TYR:CE1	1:B:212:LEU:O	2.69	0.45
1:A:161:LYS:HA	1:A:164:ASN:ND2	2.19	0.45
1:A:194:ASP:HB2	1:A:380:VAL:HG13	1.99	0.45
1:A:740:TRP:CD2	1:B:314:PRO:HD2	2.52	0.45
1:B:465:GLU:HA	1:B:468:GLU:HB2	1.99	0.45
1:B:539:ASN:HD22	1:B:539:ASN:C	2.19	0.45
1:A:238:GLY:C	1:A:240:LYS:N	2.70	0.44
1:A:646:ARG:HH11	1:A:646:ARG:CG	2.24	0.44
1:B:193:LYS:HA	1:B:379:ASN:OD1	2.17	0.44
1:B:197:GLN:HA	1:B:197:GLN:OE1	2.16	0.44
1:B:201:ILE:HD13	1:B:212:LEU:N	2.32	0.44
1:B:699:HIS:CD2	1:B:702:TRP:CD1	3.05	0.44
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.17	0.44
1:A:221:ALA:O	1:A:223:SER:N	2.50	0.44
1:A:238:GLY:HA2	1:A:257:VAL:HB	1.99	0.44
1:A:690:VAL:CG2	1:A:698:ARG:HG2	2.47	0.44
1:B:340:ALA:O	1:B:343:GLU:HB2	2.17	0.44
1:B:610:ASP:HB3	1:B:613:GLU:CG	2.47	0.44
1:A:143:THR:O	1:A:147:LEU:HG	2.17	0.44
1:A:307:ASP:OD1	1:A:309:TYR:N	2.48	0.44
1:B:348:ASN:ND2	1:B:348:ASN:N	2.65	0.44
1:A:349:MET:CG	1:A:367:THR:HA	2.45	0.44
1:A:580:ILE:HG23	1:A:583:LEU:HB2	1.99	0.44
1:A:547:TYR:HD1	1:A:696:PRO:O	1.99	0.44
1:B:233:VAL:HG12	1:B:234:HIS:N	2.33	0.44
1:B:733:ASN:O	1:B:734:GLN:C	2.56	0.44
1:B:677:ARG:HE	1:B:750:SER:HB2	1.83	0.44
1:A:122:LEU:N	1:A:122:LEU:HD12	2.32	0.44
1:A:306:GLY:HA2	1:A:461:VAL:HG22	1.99	0.44
1:A:612:GLU:O	1:A:614:TYR:N	2.50	0.44
1:B:281:ILE:N	1:B:281:ILE:HD12	2.32	0.44
1:B:404:VAL:HA	1:B:449:ILE:HG23	2.00	0.44
1:B:664:GLU:CD	1:B:664:GLU:N	2.70	0.44
1:A:262:ILE:HD11	1:A:267:LYS:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TRP:HE1	1:A:365:MET:CE	2.31	0.44
1:A:556:CYS:C	1:A:558:CYS:H	2.21	0.44
1:A:733:ASN:O	1:A:734:GLN:C	2.55	0.44
1:B:392:VAL:HG12	1:B:449:ILE:HG13	1.99	0.44
1:B:654:SER:CA	1:B:657:THR:HG22	2.47	0.44
1:A:229:THR:HB	1:A:374:LYS:HB2	1.99	0.44
1:A:343:GLU:OE2	1:A:362:THR:HG21	2.18	0.44
1:A:349:MET:HG2	1:A:367:THR:HG22	2.00	0.44
1:A:637:LEU:CD1	1:A:731:PHE:HE2	2.31	0.44
1:B:133:GLU:HA	1:B:136:ASP:HB2	2.00	0.44
1:B:508:LYS:O	1:B:512:ASN:ND2	2.51	0.44
1:B:690:VAL:CG2	1:B:698:ARG:HG2	2.47	0.44
1:A:146:LEU:O	1:A:146:LEU:HD23	2.17	0.44
1:A:300:HIS:O	1:A:301:ALA:CB	2.66	0.44
1:A:488:VAL:HG21	1:A:587:ALA:HA	2.00	0.44
1:B:309:TYR:HE2	1:B:325:ARG:CA	2.21	0.44
1:A:603:HIS:CD2	1:A:603:HIS:C	2.91	0.44
1:A:651:ARG:HH11	1:A:651:ARG:HG2	1.83	0.44
1:B:633:LYS:HD3	1:B:633:LYS:O	2.18	0.44
1:B:637:LEU:CD1	1:B:731:PHE:HE2	2.30	0.44
1:B:731:PHE:O	1:B:732:ARG:C	2.56	0.44
1:A:222:TYR:CE2	1:A:308:PRO:HG3	2.53	0.43
1:A:392:VAL:HG12	1:A:449:ILE:CB	2.49	0.43
1:A:614:TYR:HA	1:A:617:GLN:HB2	1.99	0.43
1:A:603:HIS:ND1	1:A:604:ASP:OD1	2.52	0.43
1:A:654:SER:HA	1:A:657:THR:CG2	2.48	0.43
1:A:735:LEU:C	1:A:735:LEU:HD23	2.38	0.43
1:B:180:LYS:HD2	1:B:180:LYS:H	1.83	0.43
1:B:188:VAL:HB	1:B:307:ASP:HB2	2.00	0.43
1:B:478:ALA:O	1:B:550:ILE:HD12	2.19	0.43
1:A:488:VAL:HG13	1:A:586:VAL:CG1	2.49	0.43
1:A:633:LYS:O	1:A:633:LYS:HD3	2.18	0.43
1:B:499:SER:O	1:B:501:LEU:N	2.50	0.43
1:B:565:TYR:HB3	1:B:570:MET:HB3	1.99	0.43
1:A:190:ILE:HG23	1:A:191:GLN:N	2.32	0.43
1:A:209:LEU:CG	1:A:210:VAL:N	2.76	0.43
1:A:482:ILE:HG22	1:A:483:ASN:N	2.33	0.43
1:A:721:GLN:C	1:A:723:ASN:H	2.22	0.43
1:B:238:GLY:C	1:B:240:LYS:N	2.69	0.43
1:B:513:VAL:HB	1:B:522:LEU:HD12	2.00	0.43
1:A:239:THR:O	1:A:241:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:TYR:HB3	1:B:449:ILE:HG22	2.00	0.43
1:B:513:VAL:HG22	1:B:592:GLU:HG2	2.00	0.43
1:B:582:GLU:H	1:B:582:GLU:CD	2.21	0.43
1:B:699:HIS:CD2	1:B:701:PHE:HB2	2.53	0.43
1:B:732:ARG:NH1	1:B:732:ARG:CG	2.82	0.43
1:B:735:LEU:C	1:B:735:LEU:HD23	2.38	0.43
1:A:146:LEU:C	1:A:148:ASN:H	2.22	0.43
1:A:212:LEU:O	1:A:213:VAL:C	2.55	0.43
1:A:240:LYS:C	1:A:242:ASP:N	2.69	0.43
1:A:330:PRO:O	1:A:331:ASN:CB	2.62	0.43
1:A:359:THR:CG2	1:A:360:ASP:H	2.04	0.43
1:A:564:PRO:HG2	1:A:565:TYR:CD2	2.54	0.43
1:B:146:LEU:C	1:B:148:ASN:H	2.22	0.43
1:B:204:ASP:OD2	1:B:370:SER:O	2.36	0.43
1:B:565:TYR:CD2	1:B:565:TYR:N	2.83	0.43
1:A:392:VAL:HG12	1:A:449:ILE:HG13	2.00	0.43
1:B:467:LEU:HD21	1:B:544:PHE:CZ	2.54	0.43
1:A:124:TRP:CH2	1:A:596:GLN:HG2	2.54	0.43
1:B:221:ALA:O	1:B:301:ALA:HB3	2.19	0.43
1:A:737:LEU:HD11	1:B:693:LYS:HE2	2.00	0.43
1:A:327:SER:N	1:A:329:LEU:HD12	2.34	0.43
1:A:565:TYR:CD2	1:A:565:TYR:N	2.86	0.43
1:B:201:ILE:HD12	1:B:202:ILE:H	1.81	0.43
1:B:283:MET:HG3	1:B:297:PHE:CE1	2.54	0.43
1:B:324:SER:O	1:B:325:ARG:HB3	2.19	0.43
1:A:639:LEU:O	1:A:643:TYR:CD1	2.72	0.43
1:B:488:VAL:HG13	1:B:586:VAL:HG11	2.01	0.43
1:B:603:HIS:ND1	1:B:604:ASP:OD1	2.52	0.43
1:A:610:ASP:HB3	1:A:613:GLU:CG	2.49	0.42
1:A:749:LEU:O	1:A:749:LEU:HG	2.19	0.42
1:B:232:LEU:CD2	1:B:256:ILE:HD11	2.49	0.42
1:B:730:LEU:HG	1:B:734:GLN:OE1	2.19	0.42
1:A:179:SER:O	1:A:180:LYS:C	2.58	0.42
1:A:214:GLU:OE1	1:A:341:ALA:HB2	2.19	0.42
1:A:221:ALA:O	1:A:301:ALA:HB3	2.18	0.42
1:A:309:TYR:HE2	1:A:325:ARG:CA	2.24	0.42
1:A:348:ASN:ND2	1:A:348:ASN:N	2.67	0.42
1:A:230:GLY:O	1:A:372:ASN:HB2	2.19	0.42
1:A:376:THR:HG23	1:A:376:THR:O	2.18	0.42
1:A:181:VAL:HA	1:A:391:GLY:HA2	2.00	0.42
1:B:588:ARG:HD3	1:B:589:ALA:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:ARG:CG	1:B:646:ARG:NH1	2.77	0.42
1:A:402:TYR:CD1	1:A:402:TYR:N	2.87	0.42
1:A:720:LYS:C	1:A:722:ASN:H	2.22	0.42
1:B:308:PRO:HB2	1:B:329:LEU:HD11	2.01	0.42
1:B:482:ILE:HG22	1:B:483:ASN:N	2.34	0.42
1:B:131:LEU:HD22	1:B:599:ILE:HD11	2.01	0.42
1:B:716:LEU:HD13	1:B:731:PHE:CZ	2.54	0.42
1:A:238:GLY:HA2	1:A:257:VAL:CG1	2.49	0.42
1:A:283:MET:HG3	1:A:297:PHE:CE1	2.55	0.42
1:A:467:LEU:C	1:A:469:GLY:N	2.70	0.42
1:A:588:ARG:HD3	1:A:589:ALA:N	2.34	0.42
1:A:649:PHE:O	1:A:652:ALA:HB3	2.20	0.42
1:B:204:ASP:OD1	1:B:205:LYS:N	2.43	0.42
1:B:213:VAL:HG11	1:B:345:LEU:CD2	2.47	0.42
1:B:238:GLY:HA2	1:B:257:VAL:HB	2.01	0.42
1:B:317:ASN:HA	1:B:317:ASN:HD22	1.69	0.42
1:A:198:ASN:OD1	1:A:377:VAL:HA	2.19	0.42
1:A:202:ILE:HG13	1:A:213:VAL:HG21	2.01	0.42
1:A:406:GLY:HA2	1:A:451:ALA:O	2.19	0.42
1:A:513:VAL:HB	1:A:522:LEU:HD12	2.00	0.42
1:A:754:TRP:HE3	1:A:754:TRP:HA	1.84	0.42
1:B:201:ILE:HB	1:B:212:LEU:CD1	2.49	0.42
1:B:488:VAL:HG11	1:B:583:LEU:HD12	2.02	0.42
1:B:564:PRO:HG2	1:B:565:TYR:CD2	2.55	0.42
1:A:428:LYS:HD3	1:A:428:LYS:HA	1.83	0.42
1:A:411:ALA:HA	1:A:457:ASP:OD2	2.19	0.42
1:B:353:CYS:HA	1:B:354:PRO:HD3	1.75	0.42
1:B:402:TYR:N	1:B:402:TYR:CD1	2.88	0.42
1:A:669:PHE:CE2	1:B:668:ARG:HD2	2.55	0.42
1:A:213:VAL:HG11	1:A:345:LEU:HD21	2.01	0.42
1:A:300:HIS:NE2	1:A:458:PHE:C	2.73	0.42
1:A:619:LEU:C	1:A:619:LEU:HD23	2.40	0.42
1:A:759:GLU:HG3	1:A:760:PHE:H	1.85	0.42
1:B:721:GLN:O	1:B:723:ASN:N	2.53	0.42
1:A:193:LYS:HA	1:A:379:ASN:OD1	2.20	0.42
1:A:204:ASP:C	1:A:206:ASN:N	2.71	0.42
1:A:264:PHE:O	1:A:268:VAL:HG23	2.19	0.42
1:A:307:ASP:HB3	1:A:310:THR:HG23	2.01	0.42
1:A:326:SER:N	1:A:329:LEU:HD13	2.34	0.42
1:A:514:LYS:HA	1:A:521:PHE:HA	2.00	0.42
1:A:686:LEU:HD23	1:A:699:HIS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:THR:HG23	1:B:376:THR:O	2.19	0.42
1:B:370:SER:OG	1:B:371:LYS:HG3	2.20	0.42
1:B:553:VAL:HG11	1:B:597:PHE:CD2	2.54	0.42
1:A:402:TYR:CE1	1:B:753:VAL:HG11	2.55	0.42
1:B:754:TRP:HE3	1:B:754:TRP:HA	1.84	0.42
1:A:335:GLN:NE2	1:A:336:THR:H	2.18	0.42
1:A:402:TYR:HB3	1:A:449:ILE:HG22	2.01	0.42
1:A:488:VAL:HG11	1:A:583:LEU:HD12	2.02	0.42
1:B:238:GLY:HA2	1:B:257:VAL:HG11	2.02	0.42
1:B:360:ASP:O	1:B:361:SER:O	2.38	0.42
1:B:406:GLY:HA2	1:B:451:ALA:O	2.20	0.42
1:A:145:LYS:O	1:A:148:ASN:N	2.52	0.41
1:A:232:LEU:HD13	1:A:254:ILE:HG22	2.00	0.41
1:A:614:TYR:O	1:A:618:LEU:HB2	2.20	0.41
1:A:723:ASN:HD22	1:A:723:ASN:N	2.17	0.41
1:B:193:LYS:HB2	1:B:193:LYS:NZ	2.35	0.41
1:B:349:MET:HB2	1:B:364:ARG:CB	2.50	0.41
1:A:237:PHE:O	1:A:238:GLY:C	2.59	0.41
1:A:349:MET:HA	1:A:367:THR:CA	2.50	0.41
1:A:349:MET:HB2	1:A:364:ARG:CB	2.51	0.41
1:A:568:THR:C	1:A:570:MET:H	2.23	0.41
1:A:555:PHE:CZ	1:A:594:ALA:HB2	2.55	0.41
1:A:754:TRP:NE1	1:B:449:ILE:HD12	2.35	0.41
1:B:123:TYR:O	1:B:126:ASP:HB2	2.20	0.41
1:B:221:ALA:O	1:B:223:SER:N	2.52	0.41
1:B:237:PHE:O	1:B:238:GLY:C	2.59	0.41
1:B:326:SER:N	1:B:329:LEU:HD13	2.35	0.41
1:B:667:ASP:O	1:B:669:PHE:N	2.54	0.41
1:B:699:HIS:CD2	1:B:702:TRP:H	2.36	0.41
1:A:308:PRO:HB2	1:A:329:LEU:HD11	2.01	0.41
1:A:148:ASN:HD21	1:A:416:ALA:HB2	1.86	0.41
1:B:327:SER:N	1:B:329:LEU:HD12	2.35	0.41
1:B:654:SER:HA	1:B:657:THR:CG2	2.50	0.41
1:B:721:GLN:C	1:B:723:ASN:H	2.23	0.41
1:A:180:LYS:CD	1:A:180:LYS:H	2.34	0.41
1:A:208:ARG:CD	1:A:208:ARG:O	2.63	0.41
1:A:565:TYR:HB3	1:A:570:MET:HB3	2.03	0.41
1:B:415:GLY:HA2	1:B:571:ASP:CG	2.40	0.41
1:B:386:ILE:HG22	1:B:454:SER:HB3	2.02	0.41
1:B:491:THR:HB	1:B:517:VAL:HG21	2.02	0.41
1:A:238:GLY:HA2	1:A:257:VAL:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:PRO:HG3	1:A:329:LEU:HD21	2.03	0.41
1:B:686:LEU:HD23	1:B:699:HIS:N	2.35	0.41
1:A:668:ARG:HD2	1:B:669:PHE:CG	2.55	0.41
1:A:732:ARG:HG3	1:A:732:ARG:NH1	2.28	0.41
1:A:737:LEU:C	1:A:739:THR:N	2.74	0.41
1:B:153:VAL:O	1:B:155:ARG:N	2.50	0.41
1:B:664:GLU:C	1:B:666:THR:N	2.73	0.41
1:B:709:LEU:CB	1:B:710:PRO:HD3	2.51	0.41
1:A:278:GLY:N	1:A:332:ILE:CG2	2.82	0.41
1:A:398:GLU:N	1:A:399:PRO:CD	2.84	0.41
1:B:208:ARG:H	1:B:208:ARG:HD3	1.84	0.41
1:A:740:TRP:CH2	1:B:314:PRO:HB2	2.55	0.41
1:A:188:VAL:HB	1:A:307:ASP:HB2	2.03	0.41
1:A:730:LEU:O	1:A:734:GLN:HG3	2.21	0.41
1:B:262:ILE:HD11	1:B:267:LYS:HG2	2.02	0.41
1:B:720:LYS:C	1:B:722:ASN:H	2.24	0.41
1:A:351:GLY:O	1:A:364:ARG:HB3	2.21	0.41
1:B:156:GLU:O	1:B:162:ASP:HB2	2.21	0.41
1:B:188:VAL:HG23	1:B:190:ILE:HD13	2.02	0.41
1:B:201:ILE:HD13	1:B:211:TYR:C	2.41	0.41
1:B:287:LYS:HB3	1:B:288:PHE:CD1	2.56	0.41
1:B:222:TYR:CD2	1:B:308:PRO:HG3	2.56	0.41
1:A:310:THR:OG1	1:A:465:GLU:OE2	2.38	0.41
1:A:732:ARG:CG	1:A:732:ARG:NH1	2.84	0.41
1:A:753:VAL:HG12	1:A:754:TRP:N	2.35	0.41
1:B:377:VAL:O	1:B:377:VAL:HG23	2.21	0.41
1:B:398:GLU:N	1:B:399:PRO:CD	2.84	0.41
1:B:458:PHE:HB2	1:B:461:VAL:HG21	2.02	0.41
1:B:585:LYS:O	1:B:588:ARG:HB3	2.21	0.41
1:B:691:SER:HA	1:B:692:PRO:HD3	1.98	0.41
1:B:754:TRP:HA	1:B:754:TRP:CE3	2.56	0.41
1:A:238:GLY:CA	1:A:257:VAL:HB	2.51	0.41
1:A:306:GLY:N	1:A:459:GLY:O	2.53	0.41
1:B:240:LYS:C	1:B:242:ASP:N	2.72	0.41
1:B:498:ALA:CB	1:B:553:VAL:HA	2.50	0.41
1:B:649:PHE:O	1:B:652:ALA:HB3	2.21	0.41
1:A:360:ASP:O	1:A:361:SER:O	2.39	0.40
1:B:148:ASN:HD21	1:B:416:ALA:HB2	1.85	0.40
1:B:190:ILE:HG23	1:B:191:GLN:N	2.36	0.40
1:B:514:LYS:HA	1:B:521:PHE:HA	2.02	0.40
1:B:614:TYR:HA	1:B:617:GLN:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:THR:C	1:A:511:GLN:H	2.24	0.40
1:A:758:ASN:ND2	1:A:758:ASN:N	2.66	0.40
1:B:127:LEU:CD2	1:B:127:LEU:N	2.85	0.40
1:B:307:ASP:HB3	1:B:310:THR:HG23	2.02	0.40
1:B:488:VAL:HG21	1:B:587:ALA:HA	2.02	0.40
1:B:444:PRO:CB	1:B:602:THR:HG21	2.37	0.40
1:A:280:LEU:HD22	1:A:280:LEU:N	2.36	0.40
1:A:430:ALA:HA	1:A:450:PHE:CE2	2.56	0.40
1:A:516:PRO:HG3	1:A:586:VAL:HA	2.02	0.40
1:B:351:GLY:O	1:B:364:ARG:HB3	2.20	0.40
1:B:349:MET:CG	1:B:367:THR:HA	2.48	0.40
1:B:555:PHE:HZ	1:B:594:ALA:HB2	1.87	0.40
1:A:154:PRO:HD2	1:A:161:LYS:HZ3	1.85	0.40
1:A:335:GLN:NE2	1:A:336:THR:N	2.68	0.40
1:A:404:VAL:HA	1:A:449:ILE:HG23	2.03	0.40
1:A:637:LEU:HD21	1:A:732:ARG:HE	1.85	0.40
1:B:190:ILE:CG2	1:B:191:GLN:N	2.84	0.40
1:B:298:PHE:HB2	1:B:412:TRP:CD2	2.57	0.40
1:B:719:ARG:NH1	1:B:719:ARG:CG	2.80	0.40
1:B:723:ASN:HD22	1:B:723:ASN:N	2.19	0.40
1:A:445:SER:N	1:A:602:THR:HG22	2.36	0.40
1:A:648:ASP:CG	1:A:757:ASP:OD2	2.60	0.40
1:B:278:GLY:N	1:B:332:ILE:CG2	2.84	0.40
1:B:446:ARG:NH1	1:B:602:THR:HA	2.36	0.40
1:B:467:LEU:C	1:B:469:GLY:N	2.73	0.40
1:B:698:ARG:HA	1:B:707:HIS:CD2	2.56	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	637/639 (100%)	497 (78%)	102 (16%)	38 (6%)	2	23
1	B	637/639 (100%)	498 (78%)	100 (16%)	39 (6%)	2	22
All	All	1274/1278 (100%)	995 (78%)	202 (16%)	77 (6%)	3	23

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	210	VAL
1	A	251	ASN
1	A	330	PRO
1	A	361	SER
1	A	362	THR
1	A	722	ASN
1	A	750	SER
1	A	753	VAL
1	A	759	GLU
1	B	179	SER
1	B	207	GLY
1	B	210	VAL
1	B	251	ASN
1	B	361	SER
1	B	362	THR
1	B	722	ASN
1	B	750	SER
1	B	753	VAL
1	B	759	GLU
1	A	179	SER
1	A	207	GLY
1	A	209	LEU
1	A	222	TYR
1	A	236	ASN
1	A	613	GLU
1	B	213	VAL
1	B	222	TYR
1	B	236	ASN
1	B	238	GLY
1	B	278	GLY
1	B	330	PRO
1	B	665	LYS
1	A	208	ARG
1	A	237	PHE

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Mol	Chain	Res	Type
1	A	238	GLY
1	A	239	THR
1	A	278	GLY
1	A	322	PRO
1	A	325	ARG
1	A	370	SER
1	A	558	CYS
1	A	581	PRO
1	A	665	LYS
1	B	237	PHE
1	B	322	PRO
1	B	325	ARG
1	B	581	PRO
1	A	180	LYS
1	A	566	LEU
1	B	212	LEU
1	B	239	THR
1	B	558	CYS
1	B	566	LEU
1	B	613	GLU
1	B	668	ARG
1	A	213	VAL
1	A	507	GLU
1	B	180	LYS
1	B	204	ASP
1	B	205	LYS
1	B	240	LYS
1	B	370	SER
1	B	540	ALA
1	A	153	VAL
1	A	205	LYS
1	A	569	THR
1	B	153	VAL
1	B	247	TYR
1	B	351	GLY
1	B	216	PRO
1	A	216	PRO
1	B	564	PRO
1	A	351	GLY
1	A	564	PRO
1	A	756	ILE
1	B	756	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 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	548/548 (100%)	505 (92%)	43 (8%)	15	46
1	B	548/548 (100%)	507 (92%)	41 (8%)	16	48
All	All	1096/1096 (100%)	1012 (92%)	84 (8%)	19	47

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ASP
1	A	135	LEU
1	A	148	ASN
1	A	152	TYR
1	A	153	VAL
1	A	181	VAL
1	A	197	GLN
1	A	203	VAL
1	A	204	ASP
1	A	211	TYR
1	A	224	LYS
1	A	277	ILE
1	A	310	THR
1	A	322	PRO
1	A	325	ARG
1	A	330	PRO
1	A	348	ASN
1	A	353	CYS
1	A	357	TRP
1	A	365	MET
1	A	371	LYS
1	A	418	LYS
1	A	426	LEU
1	A	446	ARG
1	A	457	ASP
1	A	525	ASP
1	A	537	LEU

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Mol	Chain	Res	Type
1	A	539	ASN
1	A	562	ASP
1	A	581	PRO
1	A	582	GLU
1	A	588	ARG
1	A	603	HIS
1	A	606	GLU
1	A	610	ASP
1	A	619	LEU
1	A	646	ARG
1	A	648	ASP
1	A	664	GLU
1	A	723	ASN
1	A	743	GLN
1	A	757	ASP
1	A	758	ASN
1	B	125	ASP
1	B	148	ASN
1	B	152	TYR
1	B	153	VAL
1	B	181	VAL
1	B	197	GLN
1	B	203	VAL
1	B	208	ARG
1	B	224	LYS
1	B	277	ILE
1	B	310	THR
1	B	322	PRO
1	B	325	ARG
1	B	330	PRO
1	B	348	ASN
1	B	353	CYS
1	B	357	TRP
1	B	365	MET
1	B	371	LYS
1	B	418	LYS
1	B	426	LEU
1	B	446	ARG
1	B	457	ASP
1	B	525	ASP
1	B	537	LEU
1	B	539	ASN

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Mol	Chain	Res	Type
1	B	562	ASP
1	B	581	PRO
1	B	588	ARG
1	B	603	HIS
1	B	606	GLU
1	B	619	LEU
1	B	646	ARG
1	B	648	ASP
1	B	660	PHE
1	B	664	GLU
1	B	723	ASN
1	B	732	ARG
1	B	743	GLN
1	B	757	ASP
1	B	758	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	160	GLN
1	A	164	ASN
1	A	191	GLN
1	A	215	ASN
1	A	275	ASN
1	A	317	ASN
1	A	335	GLN
1	A	348	ASN
1	A	408	GLN
1	A	515	HIS
1	A	539	ASN
1	A	603	HIS
1	A	662	ASN
1	A	684	HIS
1	A	699	HIS
1	A	723	ASN
1	A	758	ASN
1	B	148	ASN
1	B	160	GLN
1	B	164	ASN
1	B	191	GLN
1	B	270	ASN

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Mol	Chain	Res	Type
1	B	275	ASN
1	B	317	ASN
1	B	335	GLN
1	B	348	ASN
1	B	408	GLN
1	B	515	HIS
1	B	539	ASN
1	B	662	ASN
1	B	684	HIS
1	B	699	HIS
1	B	723	ASN
1	B	758	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](#)

There are no ligands in this entry.

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.